COUPLING CONSTRAINT BOUNDARY MAPPING IN THE PROCESS DESIGN PARAMETER SPACE WITH COMMERCIAL PROCESS SIMULATOR TO ESTIMATE PROCESS DESIGN RELIABILITY

BY

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Elim Rosalva Myers

Submitted to the graduate degree program in Chemical & Petroleum Engineering and the Graduate Faculty of the University of Kansas School of Engineering in partial fulfillment of the requirements for the degree of Doctor of Philosophy.

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ABSTRACT

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Elim Rosalva Myers

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University of Kansas, December 2009

Chemical process designs include safety factors to compensate for inherent parameter uncertainty in the design process. These safety factors require additional capital and operating expenses. Since these factors are based on rules of thumb, they may be ineffective and wasteful.

The certainty that a process will meet process constraints during normal operation despite the underlying uncertainty in process design parameters is the process design reliability. The estimation of the reliability of a proposed design and an evaluation of the safety factor effectiveness in increasing reliability would identify which equipment is unnecessarily oversized, which is critically undersized and which uncertainties are the principal contributors to low reliability. The designer could then adjust the safety factors to optimize reliability, capital investment and operating expenses.

Traditionally, reliability has been evaluated by conventional Monte Carlo integration. This methodology is computationally too expensive since it requires a large number of model simulations. Recalculation for sensitivity analysis is prohibitive. An alternative is required. Furthermore, an evaluation tool that assists designers to maximize reliability while minimizing cost would be substantially useful in a commercial process simulator.

A computationally efficient methodology for estimating reliability, Monte Carlo integration of the *c*-constraints mapped onto the *p*-parameter space, was developed, improved and coupled with a widely available commercial process simulator, CHEMCAD. In this methodology, the design's success region is mapped onto the parameter space. Sets of parameter values falling on the constraint boundary of the success region are found through process simulation coupled with a search algorithm. This search is independent of the parameter uncertainty. These boundary points are then connected via hyper-planes through interpolation. These connected hyper-planes represent a hyper-volume. Parameter sets falling within this volume successfully meet all constraints. Monte Carlo integration of the parameter uncertainty within this volume leads to an estimate of the process design reliability. This integration does not require process simulations. The procedure adds new boundary points in the regions of greatest uncertainty to improve the reliability estimate. The methodology requires two to three orders of magnitude fewer simulations than conventional Monte Carlo. The method is coupled with CHEMCAD through an EXCEL-driven central program making the method widely available to the process design community. Safety factor impact on reliability can be readily evaluated since few additional simulations are required to re-map a constraint boundary and the subsequent adjustment in the hyper-volume. Viability and efficiency are demonstrated using distillation case studies based on industrial challenges.

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SUMMARY

Chemical process designs include safety factors to compensate for inherent parameter uncertainty in the design process. However, safety factors increase capital investments and possibly operating costs. Furthermore, safety factor selection is usually little more than approximate experience-based rules-of-thumb. This is potentially wasteful and does not always eliminate design failure. The certainty that a process will meet process constraints during normal operation despite the underlying uncertainty in process design parameters is the process design reliability (PDR). An evaluation tool that assists designers to maximize PDR while minimizing cost would be substantially useful in a widely available commercial process simulator.

PDR has been traditionally estimated by conventional Monte Carlo integration (CMCI). CMCI generates sets of random numbers, Monte Carlo (MC) sets, according to the parameter probability distributions and then performs a model simulation (MS) for each set to evaluate constraint compliance. The fraction of sets satisfying the constraints is a statistical estimator of the PDR. CMCI is computationally too expensive since it requires a large number of MS's to converge to an acceptable estimate.

An alternative developed at the Kurata Thermodynamics Laboratory is the optimistic-pessimistic-tangential (OPT) procedure (MacDonald, 1993; Howat, 1995). The OPT procedure separates the model simulations from the MCI statistics, requiring

considerably less MS's than CMCI. First the OPT procedure finds few boundary points (BP's). This step requires model simulations. Then the OPT procedure geometrically interpolates among the BP's to determine the fraction of MC sets that fall within the interpolated boundary. Confidence in the reliability estimate is improved with increasing number of BP's. However as the number of BP's increases, the computational efficiency of the OPT procedure decreases.

MacDonald's (1993) developments formed the basis for the code for the CMCI and OPT procedures. The CMCI procedure was used for measuring the OPT procedure's performance. Three binary and one ternary distillation column designs were used as test problems. Uncertainties in feed flow rates, tray efficiency and thermodynamics were considered. The OPT procedure required two or three orders of magnitude fewer MS's than the CMCI procedure did.

Then modifications to the OPT procedure to improve the computational efficiency were implemented. The new procedure was called the statistically most significant direction (SMSD) procedure. While the OPT procedure uses tangential and connecting planes to interpolate between BP's, the SMSD procedures uses only connecting planes. This eliminates the MS's required to compute the tangent plane hyper-slope. .This eliminated need for the finite difference and MS's required to calculate the hyper-slope. This modification led to a new methodology for choosing the direction to search for new BP's and new criteria for defining the procedure's convergence. For testing of the SMSD procedure geometrical and distillation column design case studies were used. The SMSD procedure was able to reduce the number of MS's, but only for case studies with two uncertain parameters and specific CB's shapes.

In parallel to the testing of the SMSD procedure, the procedure was coupled with CHEMCAD using the CHEMCAD User Added Model (UAM) tool. For the coupling the SMSD procedure was coded in Visual C++ as four CHEMCAD UAM's. Once a distillation column design is developed the SMSD modules may be added to the flow sheet to estimate the PDR. For the testing of the procedure three binary distillation column designs were used. Only uncertainties in the component feed flow rates were considered. CMCI was coupled with CHEMCAD using the CHEMCAD EXCEL integration tool for comparing and evaluating the performance of the SMSD procedure. CMCI required three orders of magnitude more MS's and two to three orders of magnitude more seconds than the SMSD procedure did to the same level of reliability.

Finally a modified version of the OPT procedure was coupled with CHEMCAD using the CHEMCAD EXCEL integration tool to be used with distillation column designs with more than two uncertain parameters. Three binary and one ternary distillation column designs were used as test problems. Uncertainties in feed flow rates, tray efficiency and thermodynamics were considered. The OPT procedure required one to three orders of magnitude fewer MS's and one to two orders of magnitude fewer seconds than the CMCI procedure did to compute accurate PDR estimates. The OPT procedure required the same order of magnitude of MS's as the SMSD procedure for the three binary distillation column case studies. The OPT procedure required fewer MS's and BP's to converge than the SMSD procedure did, but the OPT procedure required few more seconds than the SMSD procedure did. The latter is attributed to EXCEL computations being slower than C++ computations and the time required for the communication between EXCEL and CHEMCAD.

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Nomenclature

Symbol	*Definition*
c	Number of process constraints
p	Number of uncertain parameters

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NOMENCLATURE

Symbol	*Definition*	*Units*
A	Counter	
$\vec{\mathbf{b}}$	[p×1] vector of constants	
B	[p×p] array with boundary points coordinates	
BA	Boundary approximation	
BP	Boundary point	
c	Number of process constraints	
c_1	Boundary approximation convergence criterion	
c_2	Boundary approximation convergence criterion	
c_3	Boundary approximation convergence criterion	
C	Scalar for checking if point is inside connecting plane approximation	
d_k	Dimensionless distance of the k-th nearest neighbor group	
D	Scalar for checking if point is inside tangential plane approximation	
E	Expected frequency	
F_i	Number of sets that fall outside de i-th nearest neighbor group statistically most significant direction	
F_i^{old}	Previous iteration value for F_i	
F_i^{new}	Current iteration value for F_i	
FT_i	Number of sets that fall outside tangential plane approximation of the i-th nearest neighbor group	
FF_i	Number of sets that fall outside connecting and tangential plane approximation of the i-th nearest neighbor group	
$\vec{g}$	Vector of process specifications or constraints	
i, j, k	Arbitrary counter variables	
L	Confidence interval length	
m	Multiplier used by line-search method	
M	Maximum statistically significant distance	
MS	Model simulation	
n	number of categories in chi-square test	
N	Sequence size, number of MC points	
N^{BP}	Number of boundary points	
N^N	Number of nearest neighbor groups	
N_i^T	Number of sets that are in the i-th nearest neighbor group	
N_k^{SO}	Number of sets outside the k-th NNG's SMSD boundary approximation	
$N_{i,j}$	Neighbor grouping for i-th group, j-th boundary point	
NNG	Nearest neighbor group	
O	Observed frequency	
p	number of uncertain parameters	
PDR	Process design reliability	
PF_i	Number of sets that fall outside either the connecting or tangential plane approximation of the i-th nearest neighbor group	

q	Ratio in neighbor grouping equation
r_i	Radial direction vector i-th coordinate
$\vec{r}$	Radial direction vector
R	Region inside constraint boundary
$\Re$	Process design reliability
$\hat{\Re}$	Process design reliability estimate
$\hat{\Re}_k$	Process design reliability estimate in previous iteration
$\hat{\Re}_{k+1}$	Process design reliability estimate in current iteration
$\hat{\Re}^O$	Optimistic process design reliability estimate
$\hat{\Re}^P$	Pessimistic process design reliability estimate
$\hat{\Re}^T$	Tangential process design reliability estimate
$\hat{\Re}^{SMSD}$	Statistically most significant direction process design reliability estimate
s_i	Number of model simulations required to find i-th boundary point
S	Total number of model simulations required
SMSD	Statistically most significant direction
$\vec{\mathbf{v}}$	[p × 1] vector for which all elements have value of one
x_i	Random number in the i-th try
$\bar{x}$	Sequence mean
z_α	Standard normal distribution critical value at the 1-α level of confidence
$Z_{\alpha/2}$	Standard normal distribution critical value at the 1-α level of confidence

Greek letters

α	Level of significance of the test
δ	One-dimensional variable to solve for in line-search method
δ_{high}	High bound of variable to solve for in line-search method
δ_{low}	Low bound of variable to solve for in line-search method
$\nabla \mathbf{g}^{Max}(\vec{\boldsymbol{\theta}}^i)$	[p×1] gradient vector of the active constraint at the i-th boundary point
ε_δ	Error criterion in line-search method
ε_g	Error criterion in line-search method
$\varepsilon_{\mathrm{OP}}$	Convergence criterion for the boundary approximation
η	Mean-square successive difference test ratio
η_h	High confidence limit
η_l	Low confidence limit
θ_i	i-th uncertain parameter
$\theta_{k,j}$	j'th coordinate of the k-th MC set
$\theta^a_{k,j}$	j'th centered coordinate of the k-th nearest neighbor group
$\theta^C_{i,j}$	j'th centered coordinate of the i-th nearest neighbor group
$\theta^C_{U,j}$	j'th centered coordinate of the nearest neighbor group with the largest PF value
θ^D_j	j'th coordinate of the nominal design point

$\vec{\boldsymbol{\theta}}$	Vector of uncertain parameter
$\vec{\boldsymbol{\theta}}^{i}$	[p×1] vector with the coordinates of the *i*-th boundary point
$\overrightarrow{\boldsymbol{\theta}^{D}}$	Nominal design point
ν	Degrees of freedom of the test
$\chi^2_{\alpha,\nu}$	Critical value of the chi-square distribution
τ	Factor used in statistically most significant direction

Mathematical and Statistical Functions

int( )	Greatest integer not greater than the argument
$\underset{i=1,\ldots,m}{Max}\{g_i\}$	Maximum value of the i-th value of vector *g*
N(μ, σ)	Normal distribution with mean μ and variance σ
Pr(·)	Probability of (·) occurring
χ^2(·)	Chi-square statistic

Chapter 1
Introduction

The design of chemical processes includes safety factors to compensate for inherent parameter uncertainty in the design process. The intention is to add some degree of flexibility to ensure that the design will be able to handle parameter variations during normal operations. However safety factors are usually little more than approximate experience-based rules-of-thumb and their use has drawbacks (Grossman and Morari, 1983; Laine and Hurme, 1994; Capps and Thompson, 1993; Howat, 1995). These are: 1) they add to capital investments and possibly to operating costs; 2) they take equipment away from the optimal operating efficiency; 3) they are often ineffective because the worst-case scenario may not be known exactly; and 4) they may even decrease the process design's likelihood to meet constraints under normal operation, i.e. process design reliability (PDR). Designers will benefit from having an evaluation procedure that helps them to maximize the PDR while minimizing costs.

Process uncertainties can be represented by a set of parameters with a range of probable values described by statistical distributions. Figure 1.1 illustrates the joint probability distributions for two uncertain parameters. The design will succeed for certain values of these parameters, i.e. all the process specifications or constraints will be satisfied. For other values the design will fail with at least one constraint violated. There are regions in the parameter space of success and failure separated by a constraint boundary. This is illustrated in Figure 1.2 for an example design with two uncertain parameters. The challenge of estimating PDR is to integrate the parameter joint probability distribution throughout the success region. The PDR is the volume under the

joint probability distribution that lies inside the process success region. In most cases joint probability distributions are unknown or they cannot be integrated beforehand. Furthermore in most cases the limits of the integrand cannot be expressed as functions of the parameters, but rather requires solving the set of non-linear equation that defines the process model. Therefore numerical integration must be used for estimating PDR.

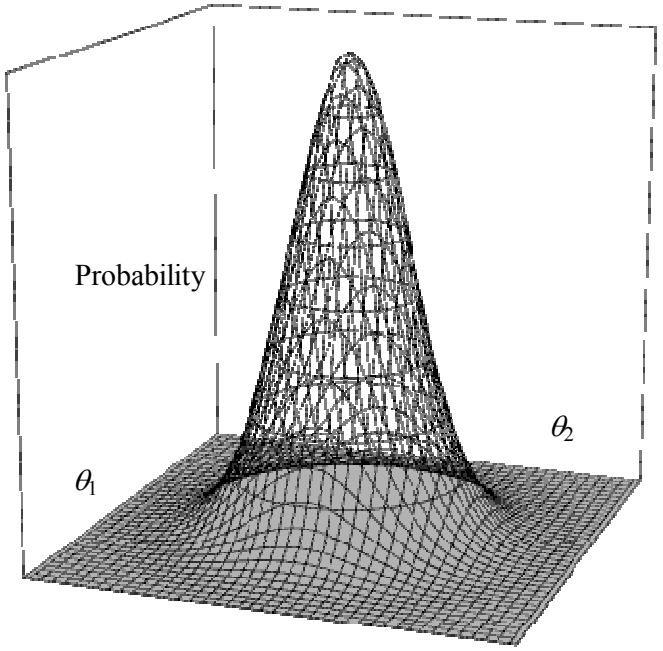

Figure 1.1. Example joint probability distribution of two uncertain parameters.

The use of statistical distributions for describing uncertainty causes unavoidable assumptions and layered uncertainties. A sensitivity analysis of the reliability can determine if these are significant. Nevertheless, if each recalculation is lengthy, a complete analysis is prohibitive.

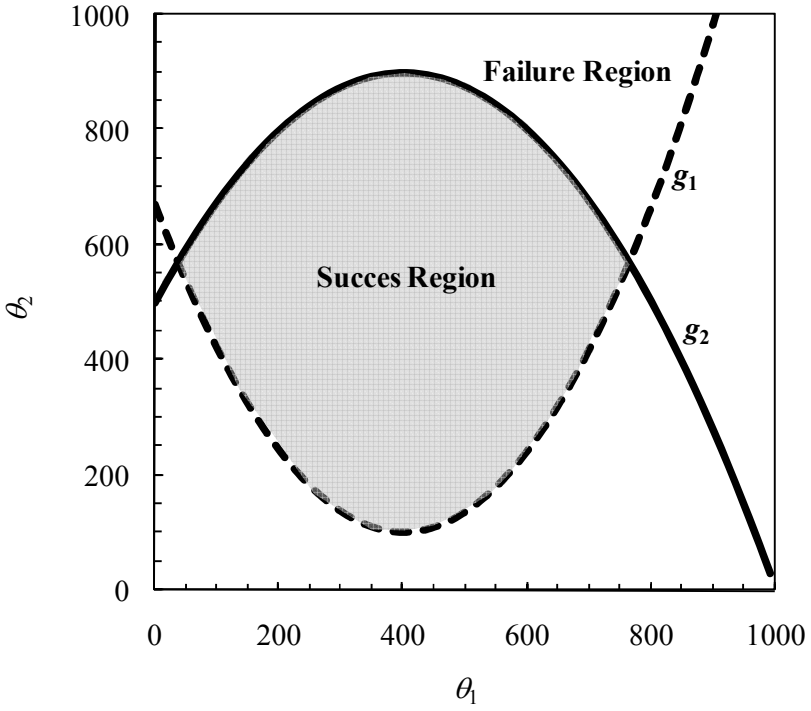

Figure 1.2. Constraint boundary in the parameter space.

In the last four decades there have been several approaches to evaluating the ability of a design to meet constraints despite the underlying design parameter uncertainty. A brief overview is presented here. Appendix C contains more literature foundation. Grossman et al. (1983), MacDonald (1993) and Bansal and Pistikopoulos (2002) present an extensive overview of different approaches. Only few approaches have considered describing the parameter uncertainty using probability distributions. Among these, many are restricted to convex, linear and/or simplified process models. Straub and Grossmann (1990 and 1993), and Pistikopoulos and Mazzuchi (1990) have developed approaches that use numerical integration based on Cartesian products. However this technique not only becomes impractical for complex geometries or high dimensions (Deák, 1988), but

also it is restricted to cases where the joint probability distribution is known. Conventional Monte Carlo integration (CMCI) does not have these restrictions and has been used by previous researches for estimating PDR (Lashmet and Szczepanski, 1974; Howat, 1983; Diwekar and Rubin, 1991). However CMCI is computationally too expensive since it requires a large number of model simulations to converge to an acceptable estimate (Howat, 1983; MacDonald, 1993; Howat, 1995).

An alternative developed at the Kurata Thermodynamics Laboratory is the optimistic-pessimistic-tangential (OPT) procedure, i.e. Monte Carlo integration (MCI) of the *c*-constraints mapped onto the *p*-parameter space (MacDonald, 1993; Howat, 1995). The computational efficiency of the OPT procedure resides in the separation of the process simulations from the statistical calculations. MacDonald (1993) demonstrated the accuracy of the OPT method and its computational efficiency by estimating the PDR of distillation columns with uncertain feed flow rates, tray efficiency and thermodynamics.

MacDonald's procedure forms the basis to meet the goals of this work. First his FORTRAN code developed in Apple operating system was modified to run in Microsoft Windows operating system. Later the procedure was modified to improve the computational efficiency. Finally two improved versions of the Monte Carlo integration (MCI) of the *c*-constraints mapped onto the *p*-parameter space were coupled with a widely available commercial process simulator to make it available to practicing engineers. The computational efficiency of the procedures was evaluated by comparing their performance versus the performance of CMCI coupled with the commercial process simulator. Binary and ternary distillation column designs were used as test problems.

Uncertainties in feed flow rates, tray efficiency and thermodynamics are described by probability statistics.

The three parts of this document are the OPT procedure, the SMSD procedure and the coupling with CHEMCAD. The results of the first section shows that the OPT method is nominally three orders of magnitude more efficient as measure by the number of model simulations than CMCI. The results of the second section show that the SMSD is substantially better than OPT for two parameters, but it is substantially worse for more. The results of the third section show that the OPT method has been integrated with CHEMCAD using a user module approach and an EXCEL-driven approach.

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Chapter 2

Accurate and Efficient Procedure for Estimating Process Design Reliability (PDR)

Abstract

All equipment includes a certain amount of contingency or safety factor because of inherent uncertainties in the design process. These increase capital costs and possibly operating costs. Safety factor selection is usually little more than approximate rules-of-thumb. This is potentially wasteful and does not always eliminate design failure. Optimal selection of safety factors requires rigorous calculation of the PDR, i.e. ability of the design to meet constraints or specifications under normal operation. Current approaches are computationally expensive. This chapter presents an efficient computational method that provides accurate and precise PDR estimates. It demonstrates the method using distillation as a test problem. Uncertainties in feed flowrates, tray efficiency and thermodynamics are described by probability statistics.

2.1. Introduction

Process designers specify equipment to perform certain tasks, e.g. chemical reactions and separations. The designer must include safety factors when sizing the equipment because of inherent uncertainties and inaccuracies in the process model and design basis (Capps and Thompson, 1983). Safety factors are traditionally based on experience embodied in rules of thumb, e.g. an additional 10% distillation trays (Walas, 1988) or sizing at 80% of distillation column flooding (Capps and Thompson, 1993). There are drawbacks in this practice:

1. They may not be effective because the worst-case scenario may not be known exactly.
2. They may decrease the ability of the process design to meet constraints or specifications under normal operation, i.e. it may decrease the PDR.
3. They move equipment operation away from the optimal operating efficiency.
4. They are not universally applicable to new technologies.
5. They are arbitrarily compounded as the design moves from simulation to specification to procurement.
6. They add to capital investments and possibly to operating costs.

Designers will benefit from having an evaluation procedure to maximize the PDR, while minimizing the capital and operating cost. This evaluation should be hierarchical. The first level is the synthesis of the proposed design. The second is the estimation of PDR and costs. The third is the identification of controlling constraints that are the principal contributors to unreliability. The designer could then adjust the safety factors accordingly and repeat the analysis until PDR and capital investment are optimized.

There are two major challenges: 1) Prohibitive computational costs in calculating PDR; and, 2) poorly developed statistical descriptions of the design uncertainties and underlying models. This chapter addresses the former.

Process uncertainties are represented by a set of parameters, $\vec{\theta}$, with a range of probable values described by statistical distributions. The design will succeed for certain values of these parameters, i.e. all the process specifications or constraints, $\vec{g}$, will be satisfied:

$$\vec{g}(\vec{\theta}) \leq 0 \qquad (2.1)$$

For other values the design will fail with at least one constraint violated. There are regions in the parameter space of success and failure separated by a constraint boundary (CB), as exemplified in the schematic shown in Figure 2.1. The challenge of the PDR estimation problem is to calculate the likelihood that the design will succeed, i.e. to integrate the parameter joint probability distribution throughout the success region. Numerical integration must be used because many joint probability distributions cannot be integrated *a priori*.

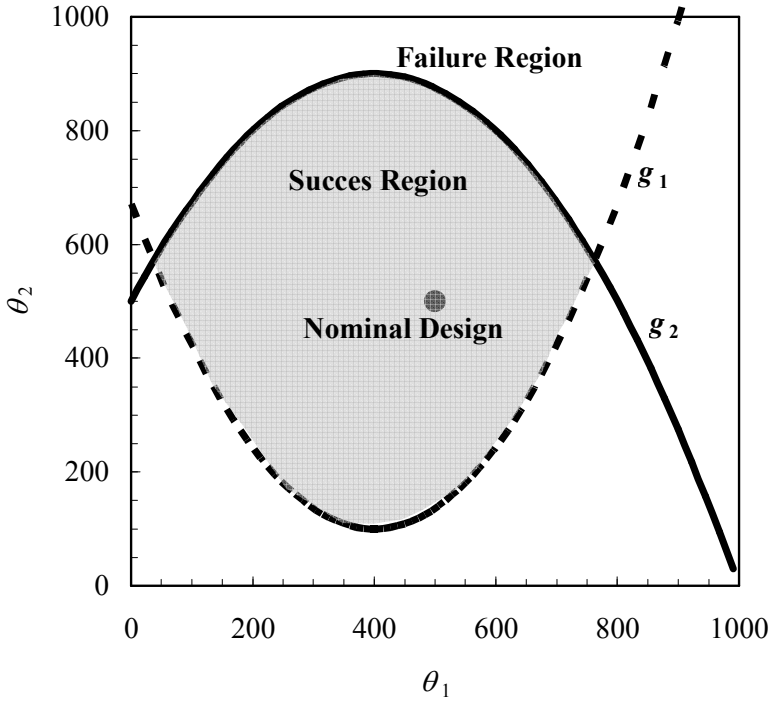

Figure 2.1. Constraint boundary in the parameter space.

Classical numerical integration based on Cartesian products, e.g. Gaussian quadrature (Straub and Grossmann, 1990, 1992; Pistikopoulos and Mazzuchi, 1990, Straub and Grossmann, 1993) or conventional Monte Carlo integration (Lashmet and Szczepanski, 1974; Howat, 1983; Diwekar and Rubin, 1991) can be used. However the former method

is limited to simple problems, e.g. Gaussian quadrature becomes impractical for complex geometries and parameter dimension greater than about five (Deák, 1988). Furthermore, classical numerical integration requires knowing the uncertain parameter joint probability distribution, which in most cases is unknown. The second option, Conventional Monte Carlo integration (CMCI), is computationally expensive. It requires hundreds of model simulations (MS's) for adequate precision and accuracy. A simplification of these two developed by Kubic and Stein (1988) calculates the probability of violating each constraint individually and then uses statistical axioms to place upper and lower bounds on the PDR. While this is computationally efficient, the bounds may be too wide to be useful (MacDonald, 1993, Howat, 1995).

A final problem in computing PDR is that statistical distributions are only equations for describing the parameter uncertainty, causing unavoidable assumptions and layered uncertainties. A sensitivity analysis of the reliability can determine if these are significant. However, if each recalculation is lengthy, a complete analysis is prohibitive.

This chapter presents a new procedure that removes each of these computational limitations by separating the MS's from the statistical calculations. It can be used with any combination of probability distributions. Sensitivity analysis can be accomplished with limited additional MS's. In this procedure, the CB's are mapped onto the parameter space. Sets of parameter values falling on the CB, boundary points (BP's), are found through MS coupled with a search algorithm. This search is independent from the parameter uncertainty. The BP's are connected through interpolation to estimate the constraint volume in the parameter space. Monte Carlo integration (MCI) of the parameter uncertainty within this volume leads to a PDR estimate. This integration does

not require MS's. The procedure adds new BP's in the regions of greatest uncertainty to improve the subsequent PDR estimate. For sensitivity analyses, the PDR is recalculated using different statistical distributions. This paper demonstrates the method using distillation as a test problem. Uncertainties in feed flow rates, tray efficiency and thermodynamics are described by probability statistics. The results prove that this method is superior to CMCI.

2.2. CMCI

CMCI is a numerical method based on random sampling. It generates sets of random numbers according to the variable probability distributions and determines whether the sets are inside or outside the domain of integration, i.e. the success region. The feature that makes CMCI superior to numerical methods based on Cartesian products is the order of magnitude of CMCI errors is independent of the dimension and does not depend on the regularity of the integrand. However CMCI can only provide a probabilistic error bound because of its stochastic nature, i.e. there is never any guarantee that the expected accuracy is achieved in a concrete calculation (Niederreiter, 1992).

A crucial task in CMCI is the generation of appropriate random samples, i.e. the success of a CMCI calculation depends on how well the random samples reflect true randomness (Niederreiter, 1992, Hellecalek, 1998). Hence, the development of the theory of computationally generated random numbers has accompanied the development of Monte Carlo methods. Variations of CMCI, quasi-Monte Carlo methods, using deterministic points instead of random points have been developed to improve CMCI accuracy and computational efficiency (Yakowitz, 1977; Deák, 1988). However, these

methods require additional effort and become complex and inefficient as the number of dimensions increases.

2.2.1. PDR estimation

Mathematically, the PDR is equal to the integration of the parameter joint probability distribution throughout the region enclosed by the constraint boundary:

$$\Re = \int_{\theta \in R} \Pr(\vec{\theta}) d\vec{\theta} = \int \ldots \int_{\theta \in R} \Pr(\theta_1, \ldots, \theta_p) d\theta_1 \ldots d\theta_p \qquad (2.2)$$

where $\Re$ is the PDR $(0 \le \Re \le 1)$, $\vec{\theta}$ is the vector of uncertain parameters and R is the region inside the CB. The region R is not known a priori. CMCI generates sets of random numbers according to the parameter probability distributions and then performs a MS at each set to determine whether or not the constraints are satisfied. The fraction of sets satisfying the constraints is a statistical estimator of the PDR.

2.2.2. Randomness and number of random numbers

Random numbers generated by any method are valid if they are uniformly distributed, statistically independent, and reproducible (Rubinstein, 1981). A good method is necessarily fast and requires minimum memory capacity. Therefore a random number generator must pass certain statistical tests to be suitable for simulation purposes. The user must be aware of the specific desirable statistical properties of the random samples to choose the appropriate tests. Several tests are available in the literature (Niederreiter, 1995; Hellecalek, 2003).

In this work two tests have been used to evaluate the adequacy of the random numbers generated by the statistical IMSL FORTRAN libraries. The chi-square goodness-of-fit test (Hogg and Craig, 1978) is used to test whether the random sample population has the expected distribution. The mean-square successive difference (Diem and Lentner, 1982) test is used to test for possible non-random influence on the mean of a normally distributed population.

The chi-square test arranges a sequence of random numbers in categories and the numbers in each category are counted. Then the observed and expected frequencies in the various categories are compared under the specified theoretical statistical distribution for the size of the random sequence. The evaluation uses the chi-square statistic:

$$\chi^2(\nu) = \sum_{i=1}^{n} \frac{(O_i - E_i)^2}{E_i} \tag{2.3}$$

where O_i and E_i are the observed and expected frequencies in the i-th category, respectively, n is the number of categories, and ν are the degrees of freedom of the test which is equal to the number of categories minus one.

The computed statistic is compared with the critical value of the chi-square distribution, $\chi^2_{\alpha,\nu}$, for a particular level of significance, α, and degrees of freedom, ν. The hypothesis that the sample population fits the theoretical statistical distribution is rejected if the computed statistic is larger than the critical value:

$$\chi^2(\nu) > \chi^2_{\alpha,\nu} \tag{2.4}$$

Figure 2.2 shows chi-square test results for three random number sequences generated by the IMSL FORTRAN libraries. The chi-square test was conducted at different sizes of the sequences. Sequence 1 and 2 are generated from normal distributions and Sequence 3

from a uniform distribution. Sequence 1 violates the 5% level of significance, i.e. 95% confidence interval (CI), for several sample sizes lower than 500, but as the sample size increases the statistic decreases leading to accept the hypothesis of randomness. The statistics for the other two sequences are lower than the critical values for all the sample sizes of the test. Then it is concluded that sequences are indeed random.

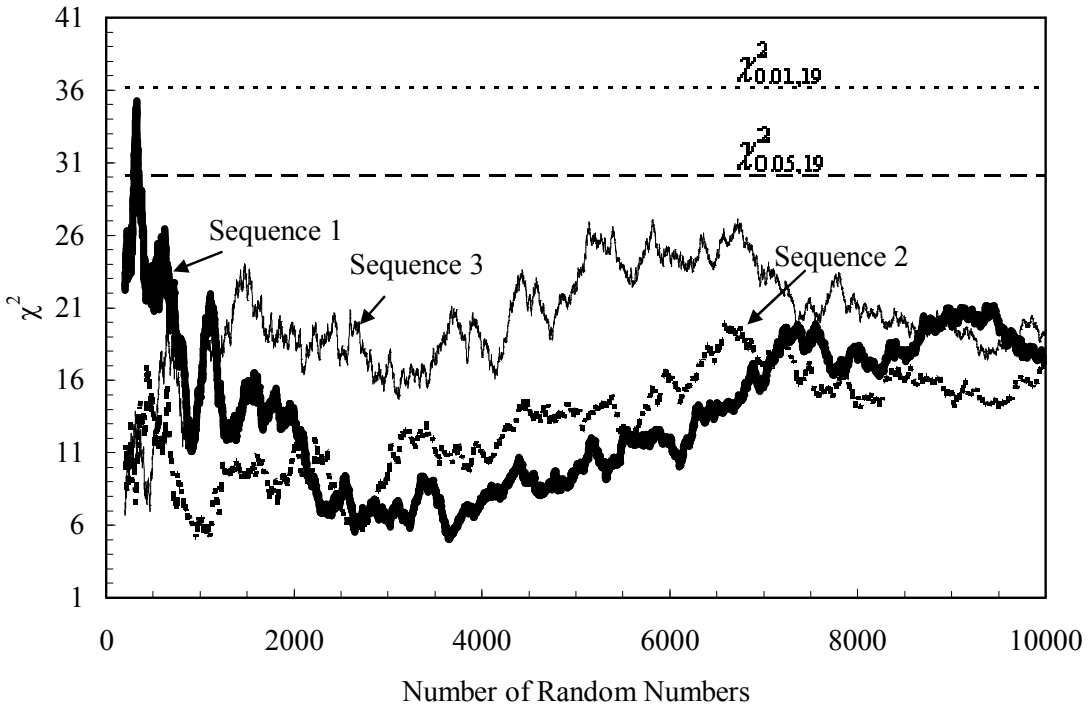

Figure 2.2. Chi-square test results as a function of the number of random numbers in the sequence.

The mean-square successive difference test computes for a sequence with normal distribution the following ratio:

$$\eta = \frac{\sum_{i=1}^{N-1}(x_{i+1} - x_i)^2}{\sum_{i=1}^{N-1}(x_i - \bar{x})^2} \tag{2.5}$$

where x_i is the random number in the i-th try, $\bar{x}$ is the sequence mean and N is the

sequence size. Confidence limits for this statistic are:

$$\eta_l, \eta_h = 2 \mp 2 z_\alpha \sqrt{\frac{N-2}{(N-1)(N+1)}} \tag{2.6}$$

where z_α is the standard normal distribution critical value at the 1-α level of confidence. If η attains or exceeds the low limit, the mean of the sequence is affected by non-random long-term factors; if it attains or exceeds the high limit, the sequence mean is affected by short-term cyclic factors. Figure 2.3 shows, at different sizes of sequence, the results for three random number sequences from normal distributions. For sequences 1 and 2 the statistic exceeds the 95% CI at a sequence size lower than 500, but stay inside the confidence limits at higher sequence sizes. Hence it is concluded that there are not significant non-random influences in the mean of the sequences.

In both tests large sequences better represent the specified distribution. Hence expected CMCI performance is better for large sequence sizes, assuming the sequence pass the randomness tests. Figure 2.4 shows the PDR estimate by CMCI as a function of the sequence size for the constraint boundary presented in Figure 2.1 and defined by the following equations:

$$g_1 = \frac{(\theta_1 - 400)^2}{280} + 100 - \theta_2 \tag{2.7}$$

$$g_2 = \theta_2 - 900 + \frac{(\theta_1 - 400)^2}{400} \tag{2.8}$$

The uncertainty in both parameters is described by the same normal distribution: N(500,100^2). 95% and 99% CI's are computed with the following equation:

$$\frac{Z_{\alpha/2}^2 + 2\hat{\Re}N \pm Z_{\alpha/2}\sqrt{Z_{\alpha/2}^2 + 4\hat{\Re}N - 4\hat{\Re}^2 N}}{2\left(Z_{\alpha/2}^2 + N\right)} \tag{2.9}$$

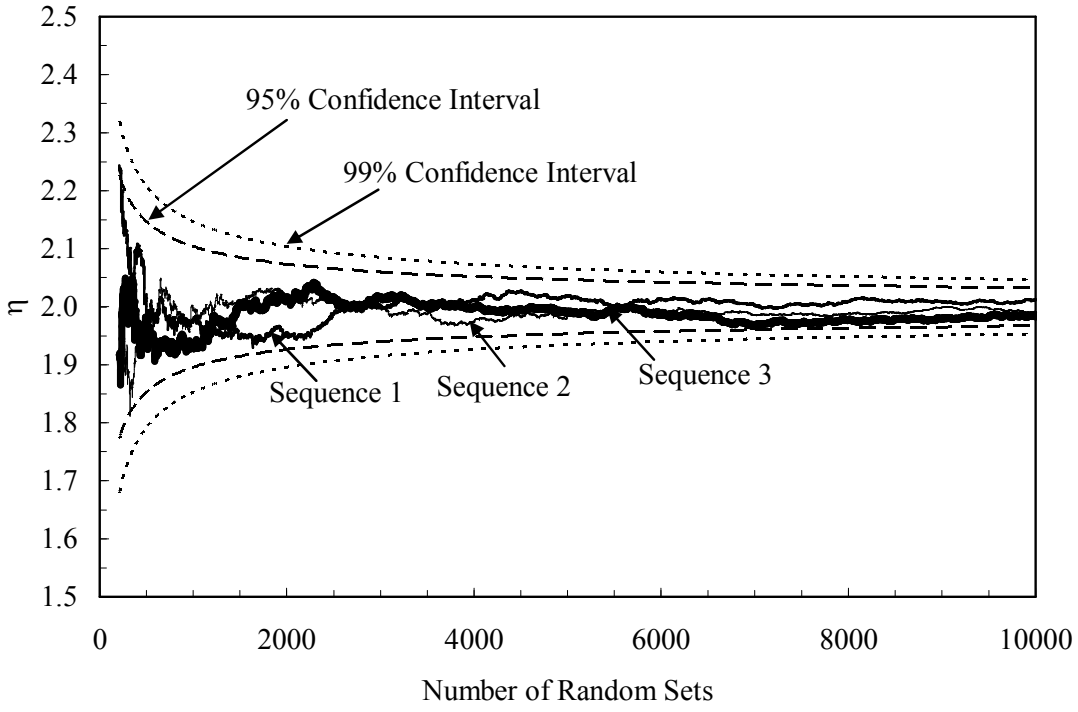

Figure 2.3. Mean-square successive difference test results as a function of the number of random numbers in the sequence.

where $\hat{\Re}$ is the estimated PDR, $Z_{\alpha/2}$ is the standard normal distribution critical value at the 1-α level of confidence and *N* is the number of random number sets. Figure 2.4 shows that an excess of over 4000 random sets are required by CMCI to converge to an accurate PDR estimate. Figure 2.5 shows the CMCI results in the parameter space. For this case study the CMCI computational effort is insignificant because no MS's are required since the constraints equations are in terms of the uncertain parameters. However, usually constraint equations are in terms of state variables for process units. Using MS, state variables are computed for a set of parameter values and hence constraints are evaluated. If the region *R* could be quickly determined by very few MS's, the CMCI procedure will become trivial. However, since this is not the case MacDonald

(1993) developed the optimistic-pessimistic-tangential (OPT) procedure to estimate PDR.

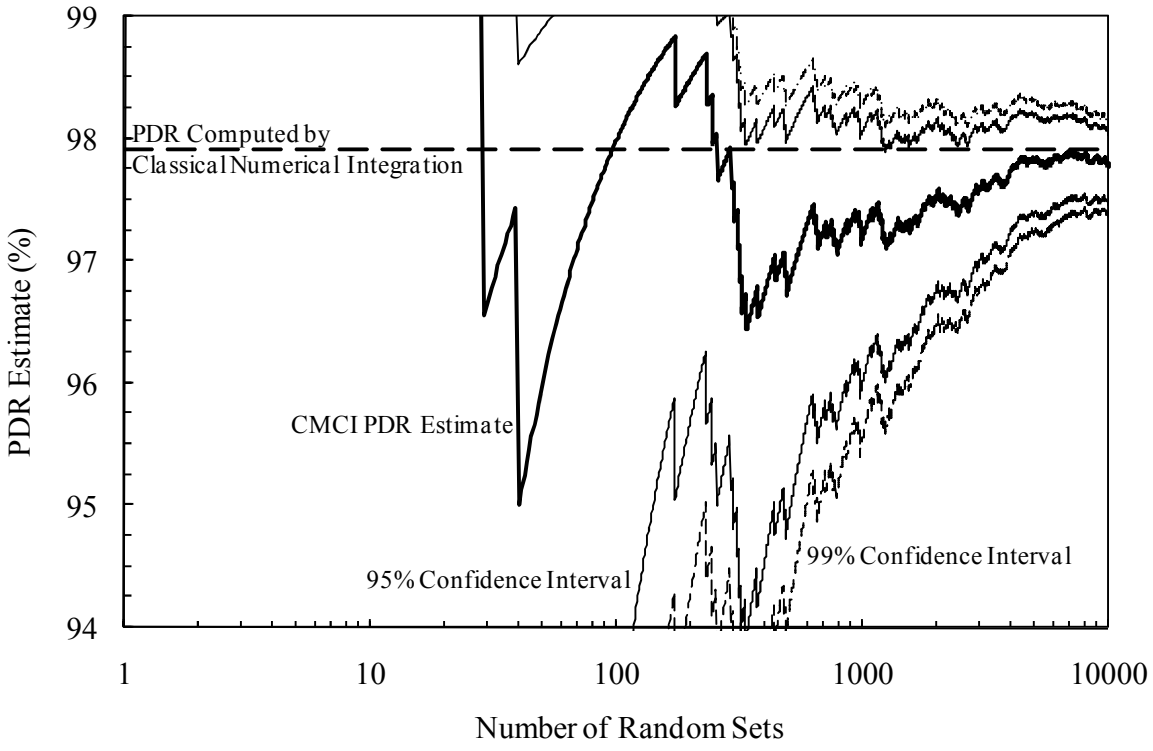

Figure 2.4. CMCI convergence to design reliability estimate as a function of the number of random sets.

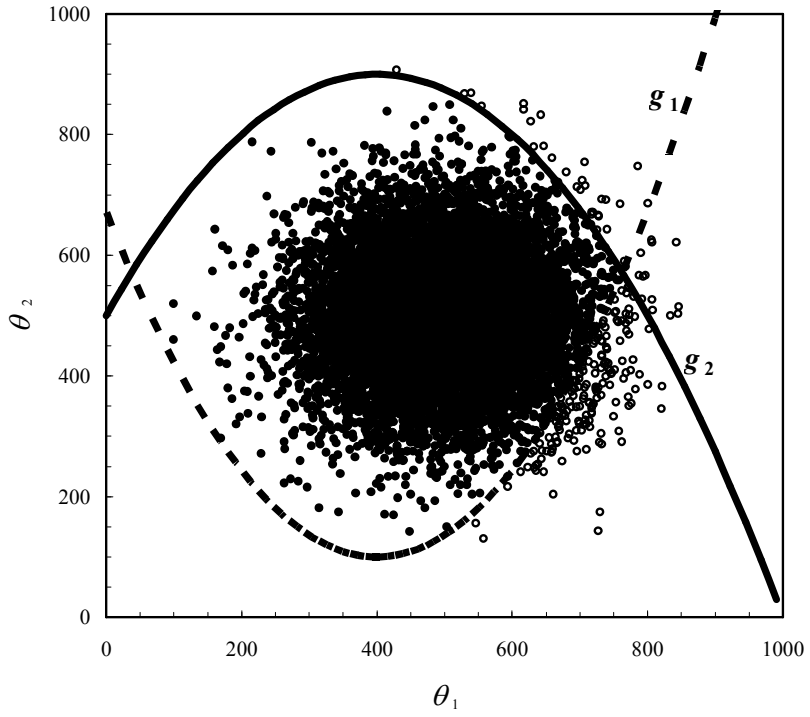

Figure 2.5. CMCI results in the parameter space shown in Figure 2.1.

2.3. OPT procedure development

The OPT procedure maps the CB by finding few BP's and then geometrically interpolating among them. Region *R* is defined as the volume included by the interpolated boundaries. The MCI procedure uses this region *R* to estimate the PDR. Interpolation is inherently inaccurate, so a balance between accuracy and number of BP's is required. An iterative approach to determine this balance is most efficient. MCI results are used to determine a new search direction to find a new BP and to evaluate the procedure convergence. The main steps of the OPT procedure are outlined in the flowchart in Figure 2.6. This flowchart shows that the MS's are separated from the MCI computations and hence the computational effort is reduced with respect to the traditional CMCI method. The steps of the procedure are described in the following sections.

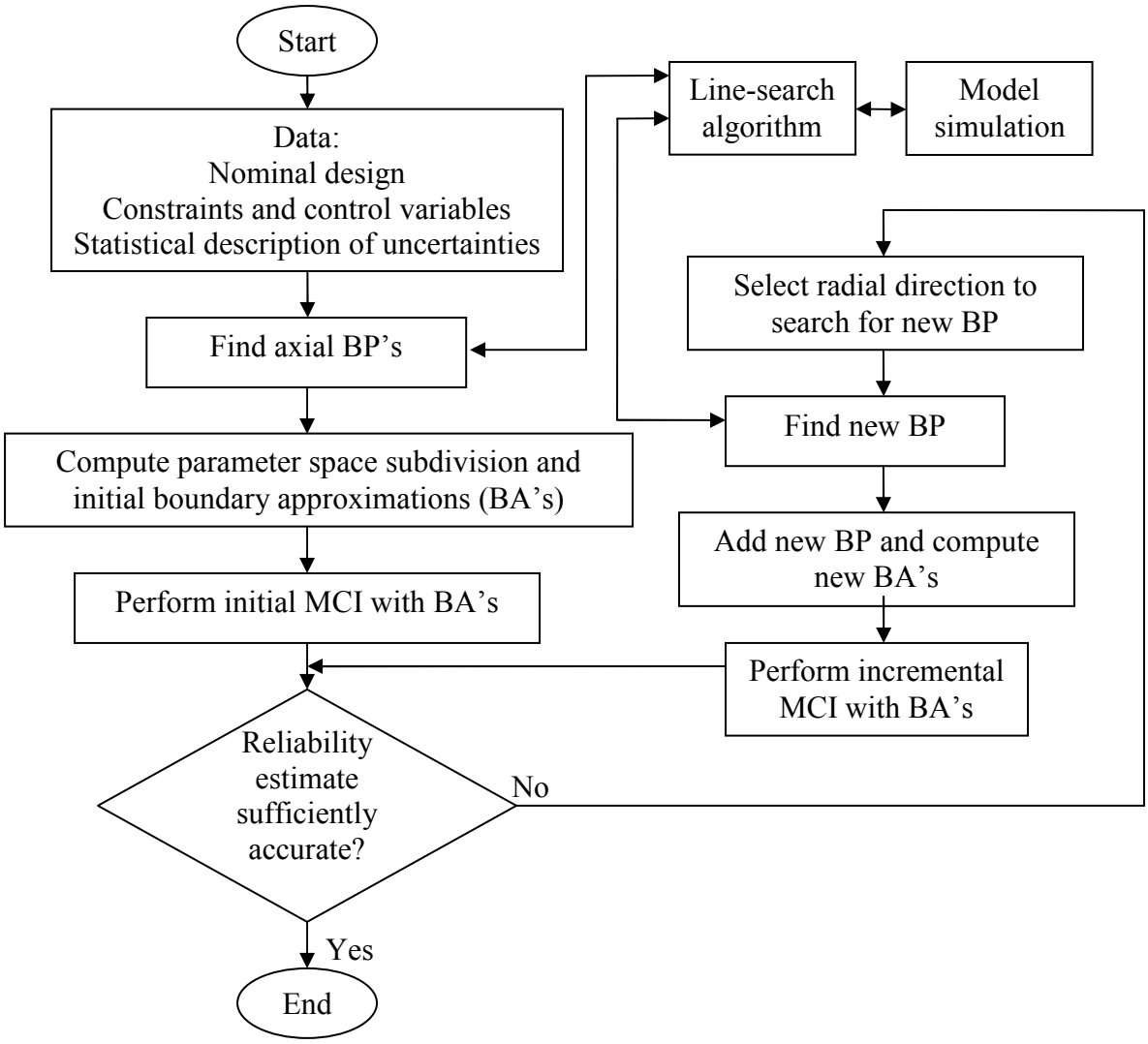

Figure 2.6. Optimistic-Pessimistic-Tangential procedure.

2.3.1. Parameter space subdivision

The entire space is subdivided into smaller, more manageable sections. This is done by organizing the parameter-space into the set of 'gaps' or *nearest-neighbor groups* (NNG's) between BP's and later developing separate local boundary approximations for each group. To ensure that the parameter space is completely covered, it is initialized with the *axial* boundary points, i.e. the set of BP's in both directions along each

parameter axis with the focal point being the nominal design point. For p parameters, there are $2p$ axial BP's. The NNG's are the set of 'gaps' between BP's. Initially, they are 2^p NNG's or hyperquadrants. Each NNG is composed of p BP's. The initial set of NNG's is created using natural neighbor sorting on the p-dimensional sphere (Watson, 1988.) First the $2p$ axial BP's are sorted by all positive directions and then all negative directions. Then Equation 2.10 provides the p BP's that compose each NNG. For the i-th NNG, its j-th BP is:

$$N_{i,j} = j + \frac{p}{2} - \left(\frac{p}{2}\right)(-1)^q \qquad i = 1,...,2^p;\ j = 1,...,p \tag{2.10}$$

where q is defined as:

$$q = \text{int}\left(\frac{i-1}{2^{p-j}}\right) \tag{2.11}$$

Here "int( )" is a function that returns the greatest integer not greater than the argument. Figure 2.7 shows the initial BP's and NNG's for case study presented in Figure 2.1. Because the parameter-space is completely covered after initialization, any additional BP must fall inside one of the existing NNG's, which subdivides the space further. When a new BP is added, it destroys the old NNG in which it falls and creates p new NNG's. The new NNG's consist of the new BP combined with p different sets of p-1 BP's from the old NNG.

The procedure defines exact borders between NNG's and uses these borders to determine in which NNG a new BP lies in. Each NNG has p sides or borders. Each border is a hyper-plane that connects p-1 BP's and the nominal design point. At initialization the borders are simply the axial planes. For instance, NNG-1 in Figure 2.7

has two borders. On border is defined by the nominal design point and point BP-1, which is the θ_1 axial direction plane. The other border is defined by the nominal design point and point BP-2, which is the θ_2 axial direction. When a new BP is added to NNG-1, the new border is defined by the new BP and the nominal design. The equations for new borders can be computed using the mathematics for connecting planes that are described in Section 2.3.3.1. For border equations the connecting points are the nominal design and the p-1 BP's that define the border. The remainder BP of a particular NNG is used as check point. A new BP or a MC set falls inside a specific NNG if it falls inside the NNG's p borders. Section 2.3.3.1 also explains the mathematics for checking if a point falls inside a border, i.e. hyper-plane.

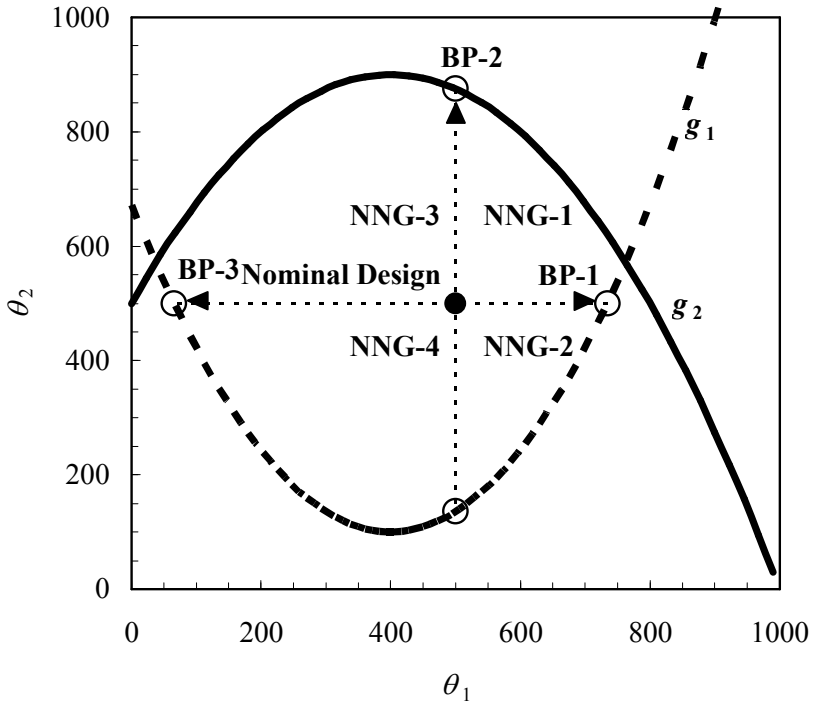

Figure 2.7. Initial parameter space subdivision for case-study shown in Figure 2.1.

2.3.2. Line-search algorithm

The line-search algorithm searches for a BP along a pre-specified radial vector, $\vec{r}$. The origin of this radial vector is the nominal design point, $\overrightarrow{\boldsymbol{\theta}^D}$. At the beginning of the OPT procedure this radial vector becomes the axial radial directions with a maximum distance of *M* times the standard deviation of the uncertain parameter in turn. *M* is generally equal to three or four. In the following OPT procedure's iterations the new radial vector is computed from the MCI statistics.

The search-path to find a BP can be represented by the equation:

$$\vec{\boldsymbol{\theta}} = \overrightarrow{\boldsymbol{\theta}^D} + \delta\vec{r} \quad ,0 \le \delta \le 1 \tag{2.12}$$

where δ is a scalar to be varied until convergence, i.e. until at least one of the boundary constraints is equal to zero. The first iteration of the line-search procedure uses the bisection method with root-bracketing values being $\delta_{low} = 0$ and $\delta_{\text{high}} = 1$. $\delta_{low} = 0$ corresponds to the nominal design point and $\delta_{\text{high}} = 1$ corresponds to the farthest significant distance from the nominal design. For subsequent iterations the Regula-Falsi method is used to compute a new value for δ and select new bracketing values. When the computed δ from the Regula-Falsi equation is too close to one of the bracketing values, one of the following equations is used to recomputed δ and speed up the convergence to the solution:

$$\delta = \delta_{low} + 1.5 \times \left(\delta - \delta_{low}\right) \text{ if } \frac{\delta - \delta_{low}}{\delta_{high} - \delta_{low}} \le 0.30 \tag{2.13}$$

$$\delta = \delta_{high} - 1.5 \times \left(\delta_{high} - \delta\right) \text{ if } \frac{\delta_{high} - \delta}{\delta_{high} - \delta_{low}} \le 0.30 \tag{2.14}$$

Convergence is achieved when either one of the two following criteria is satisfied:

$$\delta_{high} - \delta_{low} < \varepsilon_{\delta} \tag{2.15}$$

$$\left| \underset{i=1,\ldots,c}{Max}\{g_i\} \right| < \varepsilon_g \tag{2.16}$$

It may be possible, that in a radial direction, a BP does not exist between the maximum distance and the nominal design. This is determined in the first iteration of the line-search procedure from the constraint values at the maximum distance from the nominal design. If the constraint with the maximum value is less than zero, the point is inside the constraint boundary. The point is tagged as a "non-failure point" and the search stops.

2.3.3. Interpolations

The OPT procedure uses two geometrical interpolations to build constraint boundary approximations (CBA's): connecting and tangential planes.

2.3.3.1. Connecting plane mathematics

The connecting plane boundary for each neighbor group is the hyperplane connecting the *p* points of that group. Since there are *p* points in *p*-space, the solution is unique and can be solved by the following equation:

$$\vec{\mathbf{b}} = -\mathbf{B}^{-1}\vec{\mathbf{v}} \tag{2.17}$$

where $\vec{\mathbf{b}}$ is the [p×1] vector of constants; **B** is a [p×p] array with the coordinates of the boundary points that compose the nearest neighbor group, the *i*-th row being the coordinates of the *i*-th point; and $\vec{\mathbf{v}}$ is a [p × 1] vector for which all elements have the value of one. The result *C* in Equation 2.18 must be negative if a point $\vec{\boldsymbol{\theta}}$ falls "inside" the NNG volume defined by the volume included by the plan and the design point:

$$C = \vec{\mathbf{b}}^{T}\,\vec{\boldsymbol{\theta}} + \vec{\mathbf{v}} \tag{2.18}$$

$\vec{\boldsymbol{\theta}}$ is a [p×1] vector with the coordinates of the point. Because the nominal design is always inside all the connecting planes, it is used as check point in Equation 2.18. If the result *C* of this operation is positive, $\vec{\mathbf{b}}$ must be multiplied by minus one before it can be used for building the boundary approximation. Figure 2.8 shows the connecting planes for the initial BP's of the case presented in Figure 2.1.

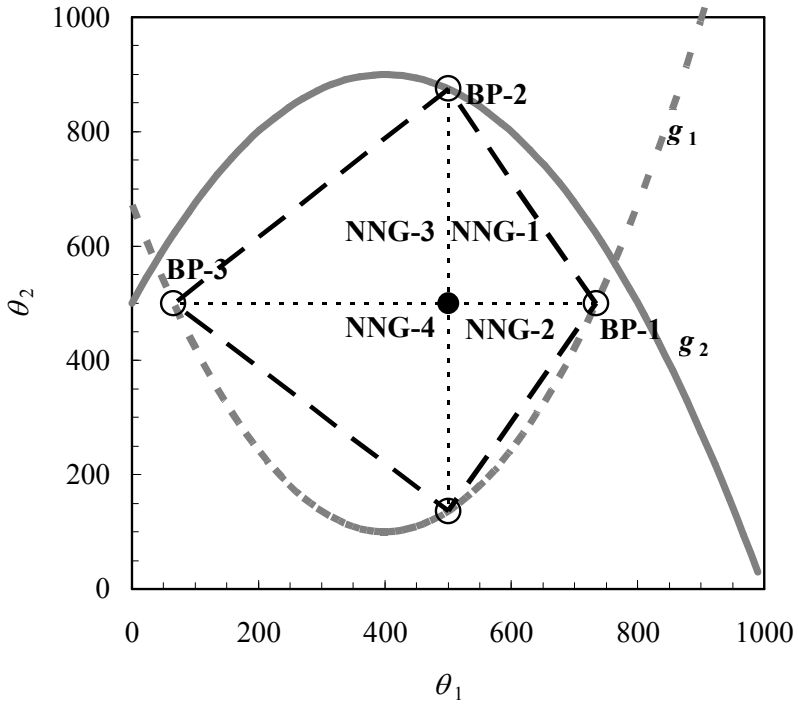

Figure 2.8. Initial connecting planes for case-study shown in Figure 2.1

2.3.3.2. Tangential plane mathematics

The tangential plane for each NNG is made up of the intersection of the individual tangent-planes at each BP of that group. The equation for each individual BP tangent-plane is:

$$\left(\nabla \mathbf{g}^{Max}(\vec{\boldsymbol{\theta}}^{i})\right)^{T}\left(\vec{\boldsymbol{\theta}}-\vec{\boldsymbol{\theta}}^{i}\right)=0 \tag{2.19}$$

where $\vec{\boldsymbol{\theta}}^{i}$ is the [p×1] vector with the coordinates of the *i*-th BP, $\vec{\boldsymbol{\theta}}$ is the [p×1] vector containing the coordinates of a point that falls on the tangent-plane and $\nabla \mathbf{g}^{Max}(\vec{\boldsymbol{\theta}}^{i})$ is the [p×1] gradient vector of the active constraint, $\underset{i=1,\ldots,m}{Max}\{g_i\}$, at BP $\vec{\boldsymbol{\theta}}^{i}$ with elements:

$$\left(\nabla \mathbf{g}^{Max}(\vec{\boldsymbol{\theta}}^{i})\right)^{T}=\left[\frac{\partial g^{Max}}{\partial \theta_1^i},\ldots,\frac{\partial g^{Max}}{\partial \theta_p^i}\right] \tag{2.20}$$

These elements are computed by finite differences for each BP after the line-search algorithm has converged for any BP. For "non-failure" points there is no evaluation of the tangent and hence they are not used for building the tangential plane. Figure 2.9 shows the initial tangent-planes for the case presented in Figure 2.1.

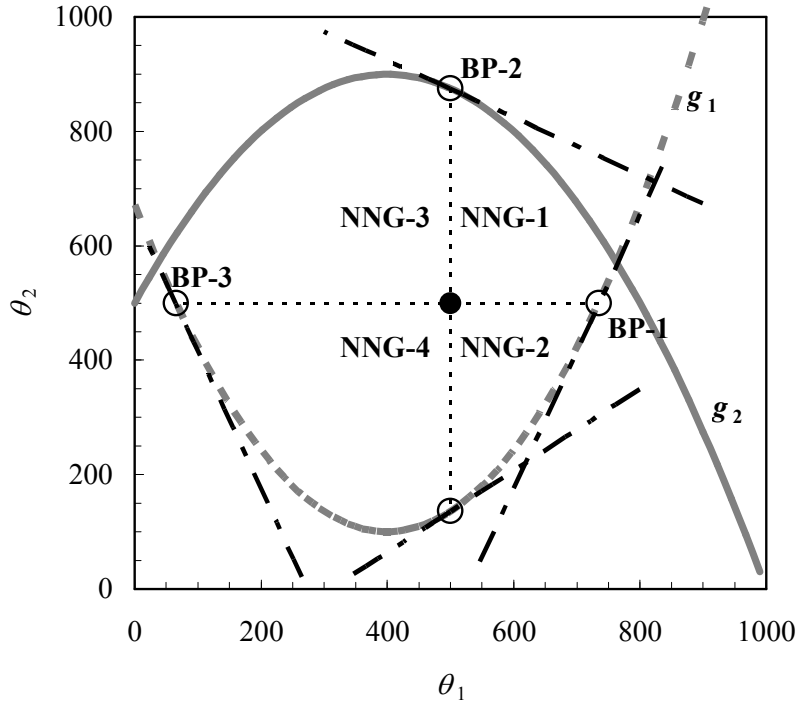

Figure 2.9. Initial tangential planes for case-study shown in Figure 2.1

2.3.4. Boundary approximations

The OPT procedure builds three CBA's using the connecting and tangential planes: tangential, optimistic and pessimistic approximations. The tangential approximation uses only the tangent-planes. The construction of the optimistic and pessimistic boundary approximations depend upon the curvature of the actual CB at each NNG. An algorithm to determine the NNG curvature checks if all its BP's fall or not inside all its individual tangent-planes. Depending upon the results the NNG curvature may be convex, concave or saddle. To determine if a point $\vec{\boldsymbol{\theta}}$ falls inside the individual tangent-plane of the *i*-th BP the following equation is used:

$$D = \left(\nabla \mathbf{g}^{Max}(\vec{\boldsymbol{\theta}}^{\,i}) \right)^T \left(\vec{\boldsymbol{\theta}} - \vec{\boldsymbol{\theta}}^{\,i} \right) \tag{2.21}$$

here the result D must be negative if the point falls inside the tangent-plane. The algorithm is outlined in the flowchart shown in Figure 2.10.

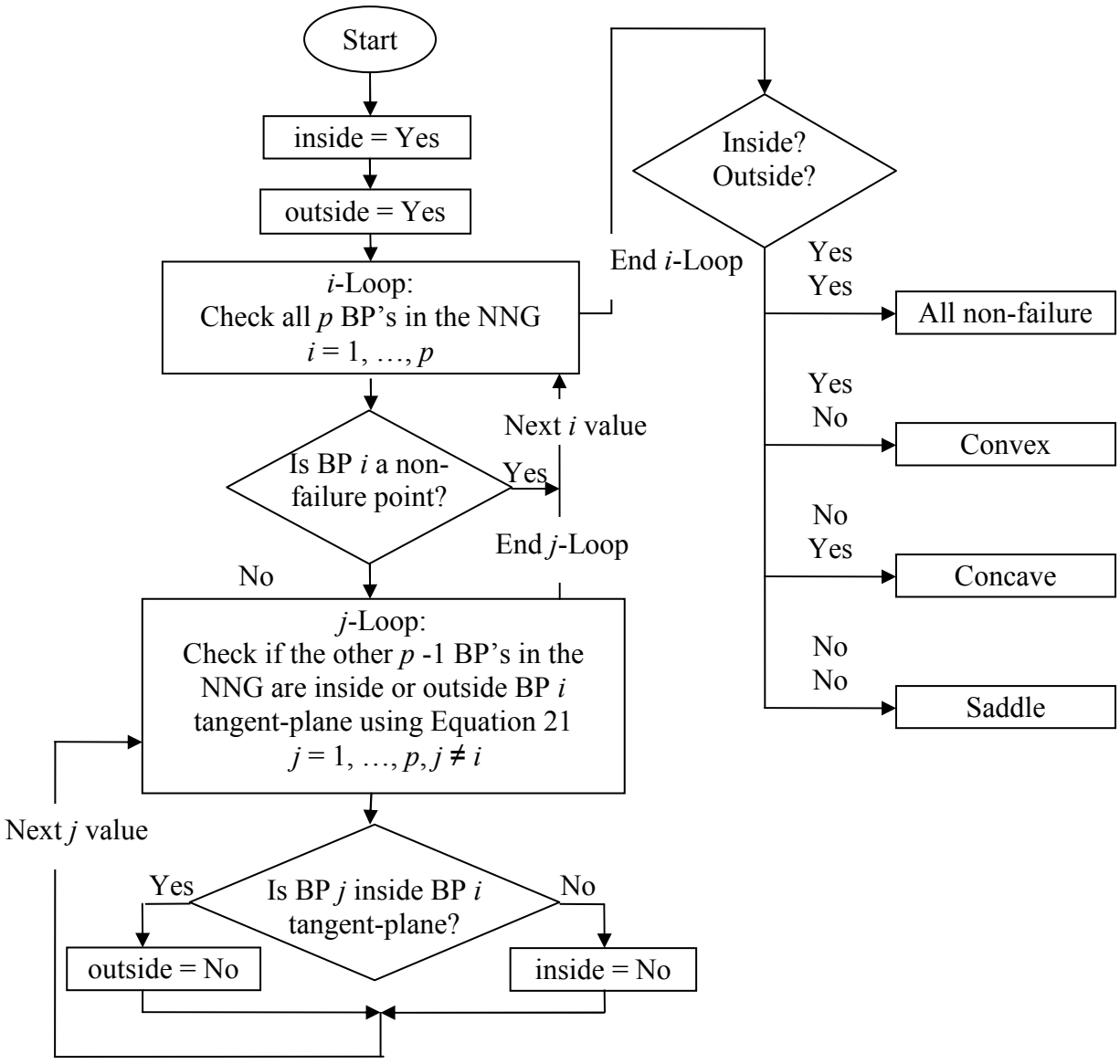

Figure 2.10. Flowchart of the procedure to determine the constraint boundary curvature in a specific NNG.

If the NNG curvature is convex the connecting plane is a pessimistic approximation of the actual constraint boundary and the tangential plane in an optimistic approximation.

By pessimistic, the volume enclosed by the planes is the smallest of the computed volumes and presumed to be smaller than the true volume. This can be observed in all the NNG's of the example in Figure 2.8. However if the NNG curvature is concave the connecting plane is an optimistic approximation and the tangential plane a pessimistic approximation. The latter case is represented in the example shown in Figure 2.11.

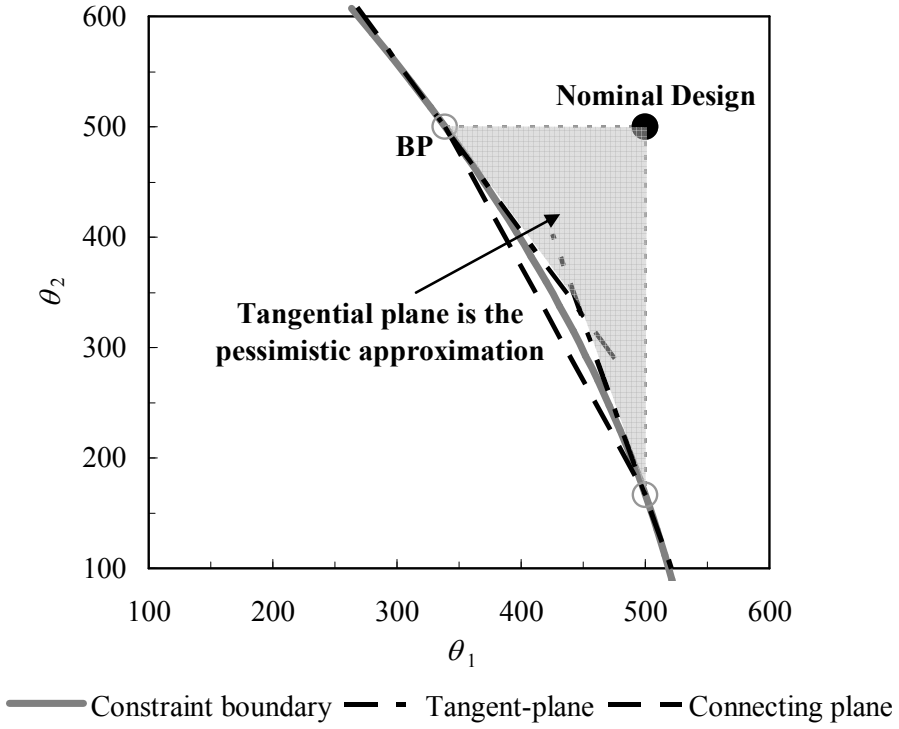

Figure 2.11. Schematic showing a NNG with concave curvature, the tangential plane is the pessimistic approximation and the connecting plane the optimistic approximation.

If the NNG curvature is saddle the individual tangent-planes of the BP's in the NNG may not intersect inside the NNG region or may introduce large error in the boundary approximation. A reasonable approach to define the tangential plane is by a "discontinuous" tangential plane that results from using the tangent-plane that is nearest to the region that is being approximated as it is shown in Figure 2.12. The step change in

between tangent-planes is inaccurate, but at least it occurs in the region of greatest uncertainty in the NNG, i.e. farthest from any BP. The resulting CBA's cannot be rigorously optimistic or pessimistic but a combination of them. For instance, for the example presented in Figure 2.12 one of the tangent-planes is an optimistic approximation of the actual constraint boundary and the other is a pessimistic approximation. Also for Figure 2.12, the connecting plane results in an optimistic approximation of the actual constraint boundary in one region of the NNG and a pessimistic approximation in the rest of the NNG region.

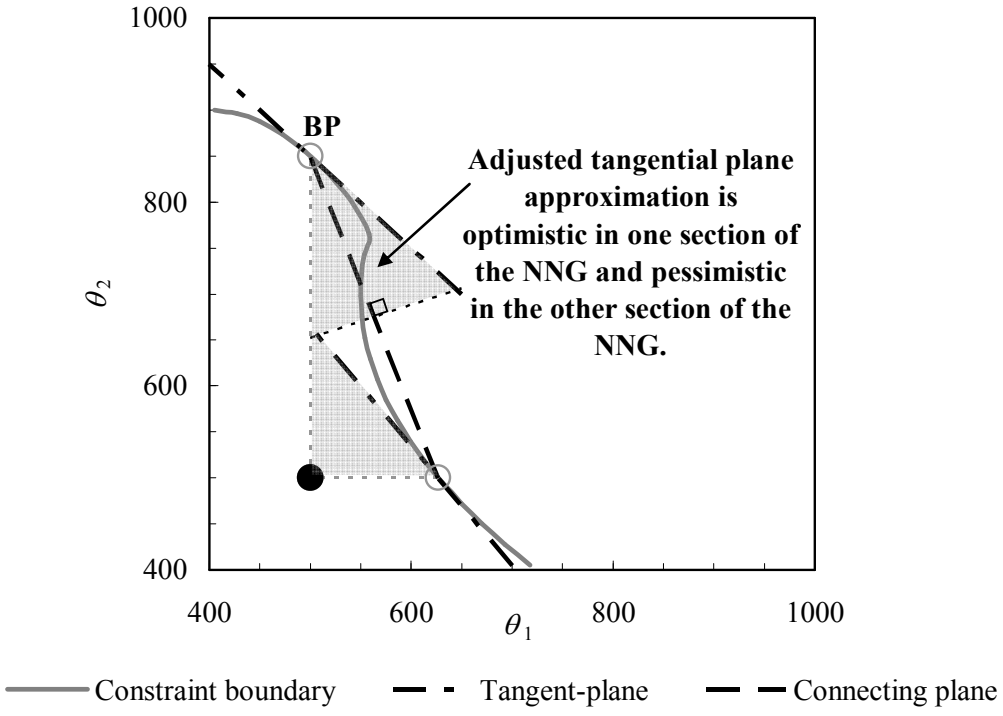

Figure 2.12. Schematic showing NNG with "saddle" curvature.

2.3.5. MCI

The OPT procedure computes three PDR estimates by MCI using the pessimistic, optimistic, and tangential CBA's. Sets of random points are generated by the MCI procedure. As each random point is generated, it is first examined to find the NNG in which it resides. Then the point is checked to see if it is inside or outside the connecting plane and tangent-planes of the particular NNG using Equations 2.18 and 2.21 as indicated in the flow chart shown in Figure 2.13. The sequence of the steps varies depending upon the NNG curvature.

The MCI procedure keeps track of the number of points that fall inside each NNG, N_i^T, and the number of points for each NNG that fall: 1) outside the tangential approximation, FT_i; 2) outside either the connecting plane or the tangential plane but not outside of both, PF_i, 3) outside both the connecting plane and the tangential plane, FF_i. The optimistic, pessimist, and tangential PDR estimates, $\hat{\Re}^O$, $\hat{\Re}^P$, and $\hat{\Re}^T$ respectively, are computed as percentages:

$$\hat{\Re}^O = 100N^{-1}\sum_{i=1}^{N^N}\left(N_i^T - FF_i\right) \tag{2.22}$$

$$\hat{\Re}^P = 100N^{-1}\sum_{i=1}^{N^N}\left(N_i^T - FF_i - PF_i\right) \tag{2.23}$$

$$\hat{\Re}^T = 100N^{-1}\sum_{i=1}^{N^N}\left(N_i^T - FT_i\right) \tag{2.24}$$

where N^N is the number of NNG's and N is the number of MC points. MCI results for the initial NNG's of the case presented in Figures 2.1, 2.5, 2.7, 2.8 and 2.9 are presented in Figure 2.14. The initial tangential approximation is not indicated because for this case it is the same as the optimistic approximation. The random points that fall inside one of the

CBA's but not inside the other, in Figure 2.14 light-grey points with no black point in the center, represent the uncertainty in the CBA.

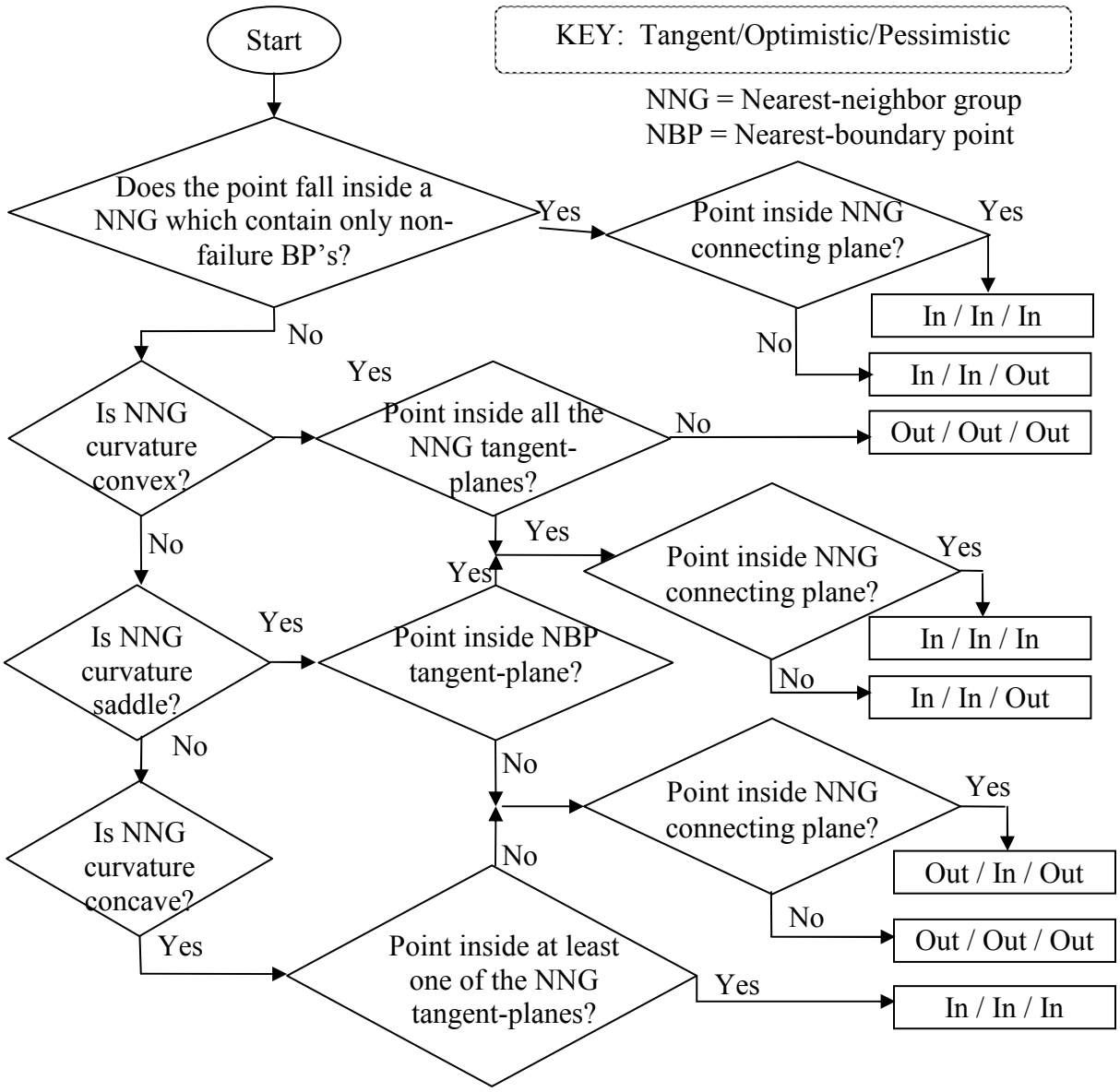

Figure 2.13. Flowchart of the procedure to determine if a random point falls inside or outside the constraint boundary approximations of a specific NNG.

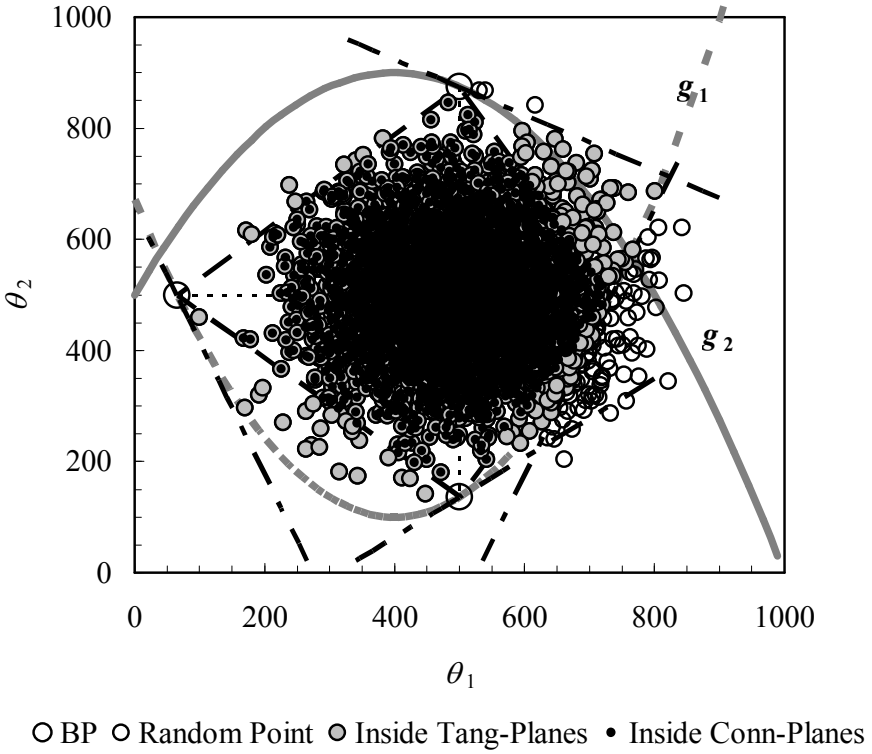

Figure 2.14. MCI results for initial NNG's.

2.3.6. New search direction and incremental MCI

The difference between the optimistic and pessimistic PDR estimates serves as a measure of uncertainty of the constraint boundary approximations. Reducing that difference would make the boundary approximation converge to the actual constraint boundary. Each NNG has its own region of uncertainty. The statistical significance of that region is proportional to the number of MC points that fall within it. Therefore, the group with the largest *PF* value, is selected as the NNG where a new BP must be found to improve its boundary approximations. A radial direction vector, $\vec{\mathbf{r}}$, must be identified to search for the next BP within the NNG. The vector points towards the region where the MC points are concentrated, i.e. the most statistically significant region.

Mathematically, this is accomplished by averaging the location of the Monte Carlo points to provide a 'centered' location. The MCI procedure keeps track of this centered location for all the NNG's:

$$\theta_{i,j}^{C} = \frac{\sum_{k=1}^{PF_i} \theta_{k,j}}{PF_i}, \quad i = 1,2,...,N^N;\ j = 1,2,...,p \tag{2.25}$$

where $\theta_{k,j}$ is the j'th coordinate of the k-th MC point that falls in the region of uncertainty of the i-th NNG. The radial vector is computed with respect to the nominal design position by:

$$r_j = m \times \left(\theta_{U,j}^{C} - \theta_j^{D}\right) \quad j = 1,2,...,p \tag{2.26}$$

where U refers to the NNG with the largest PF value and m is a multiplier. This multiplier is used to obtain a vector with magnitude equal to the maximum statistically significant distance. This maximum statistically significant distance is equal to M times the combined standard deviations of the uncertain parameters. For additional BP's M is generally equal chosen to be three, but it may take any value between three and four. For example, for a design case with two uncertain parameters defined by two independent normal distributions N(μ_1, σ_1) and N(μ_2, σ_2), the multiplier is computed by:

$$m = \frac{M}{\sqrt{\left(\frac{\theta_{U,1}^{C} - \theta_1^{D}}{\sigma_1}\right)^2 + \left(\frac{\theta_{U,2}^{C} - \theta_2^{D}}{\sigma_2}\right)^2}} \tag{2.27}$$

After the radial vector is computed the linear-search procedure finds the new BP.

The new BP is used to form p new NNG's and the old NNG disappears. Connecting and tangential planes are constructed for the new NNG's. Because the same sets of random points are used for the MCI, it is only necessary to perform the computations for

the sets that fall inside the new NNG's, which is named incremental MCI in the flowchart in Figure 2.6. Figure 2.15 shows the PDR estimates as a function of the number of BP's that are added to the boundary approximation and Figure 2.16 shows the estimates as a function of the number of MS's. The optimistic and tangential estimates, which are the same for this example, start with a more accurate value than the pessimistic estimate. After six BP's the optimistic and tangential estimates do not change significantly. The error in the pessimistic estimate for six BP's is 3%. Increasing the number of BP's to 10 with almost triple the number of MS's reduces the error in the pessimistic estimate to 0.3%. Figure 2.16 shows how the OPT procedure reduces significantly the computer effort required by CMCI.

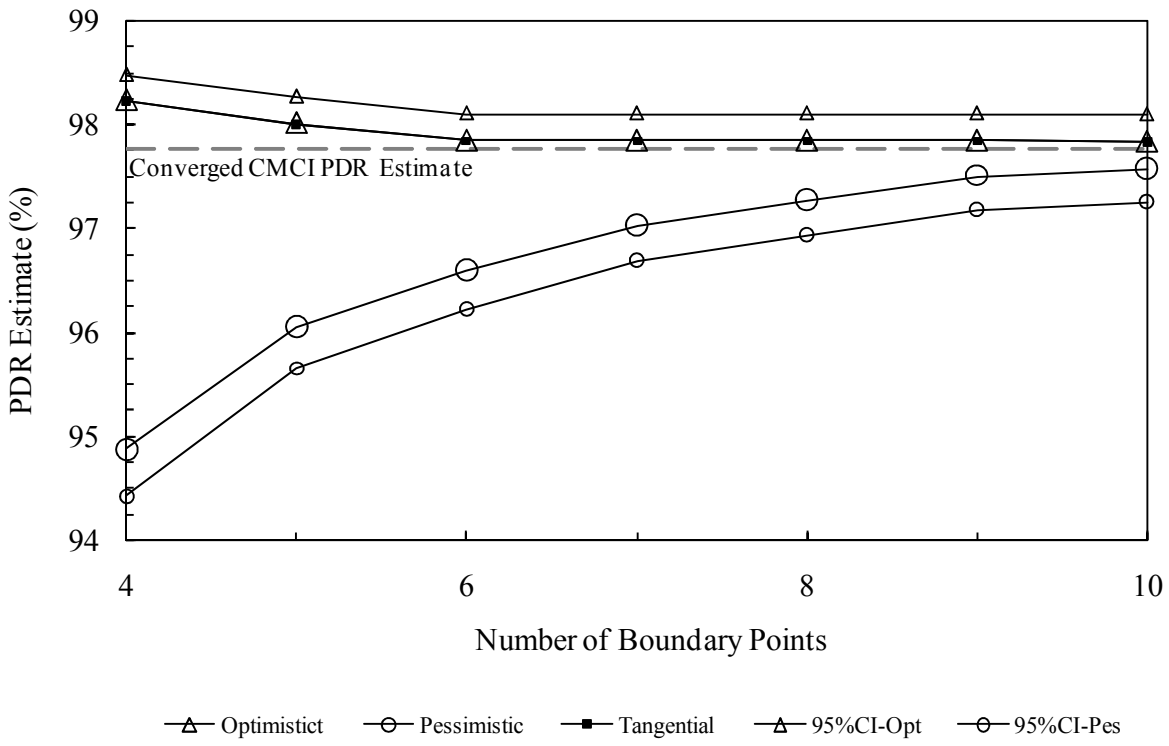

Figure 2.15. PDR estimate as a function of the number of BP's estimated by OPT procedure.

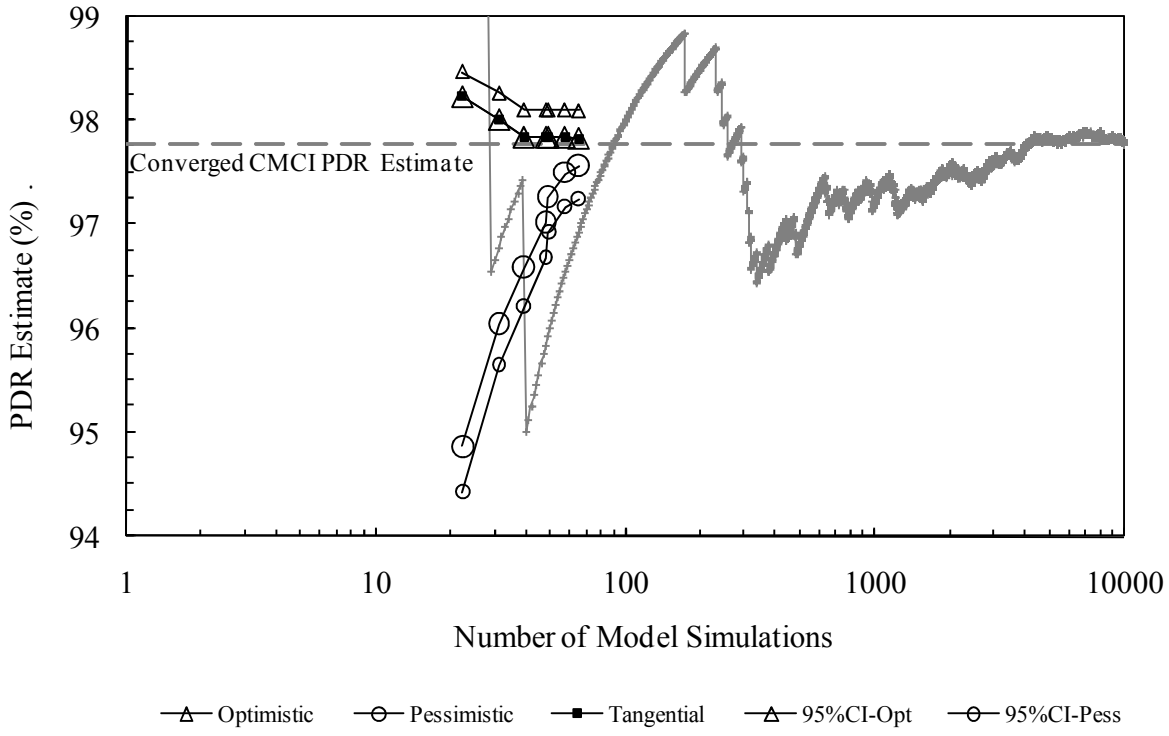

Figure 2.16. PDR estimate as a function of the number of MS's estimated by OPT procedure.

2.3.7. Convergence of the CBA

Desirable convergence is reached when the difference between the optimistic and pessimistic estimates is sufficiently small:

$$\left|\hat{\Re}^{O} - \hat{\Re}^{P}\right| \leq \varepsilon_{OP} \qquad (2.28)$$

here ε_{OP} is the acceptable uncertainty in the boundary approximation. However, as it is shown in Section 2.5, for design cases with more than two uncertain parameters the pessimistic CBA is not able to approximate accurately the CB. Because of this, for design cases with more than two uncertain parameters Equation 2.28 is not used as a measure of convergence. Other ways to evaluate the procedure's convergence is

addressed in Chapter 3. For purposes of evaluating the OPT procedures performance in this work converged CMCI PDR estimates are used. However, normally these values would not be available.

2.4. Distillation case studies

Binary and ternary distillation column designs, including wide and narrow boiling, ideal and nonideal systems are used as procedure tests. Distillation was selected because of its industrial importance and major design uncertainties. Furthermore, solution of the distillation model is computationally expensive, so it provides a realistic demonstration of the practical capabilities of the mathematical procedures. Process control variables, which give operating flexibility to meet process constraints, were set to their limiting values to reduce the burden of the problem. The parameter uncertainties included in this work are: feed component flowrates described by normal distributions, tray efficiencies described by a uniform distribution and thermodynamic binary parameters described by correlated normal distributions. Table 2.1 summarizes the distillation tests specifications.

Table 2.2 shows the PDR estimates for the case studies computed by CMCI using several random set sizes. Table 2.3 shows the estimate's 95% CI length computed by

$$L = \frac{Z_{\alpha/2}\sqrt{Z_{\alpha/2}^2 + 4\hat{\Re}N - 4\hat{\Re}^2 N}}{\left(Z_{\alpha/2}^2 + N\right)} \tag{2.29}$$

For cases with PDR's higher than 95%, random set sizes of 1,000 or less are enough to converge to an accurate PDRE. However, more than 1,000 sets may be required to reduce their CI's to an acceptable value. For cases with PDR's lower than 95%, an excess of 1,000 random sets or more are required.

Table 2.1. Distillation case-studies description.

Data \ Mixture		A/B	A/W	M/I	A/B/T
Column specifications					
Stages		25	14	200	25
Feed stage		15	8	125	15
Feed state		Sat. liquid	Sat. liquid	Sat. liquid	Sat. liquid
Condenser pressure		15 psia	15 psia	24.65 psia	15 psia
Vapor overhead		18 psia	18 psia	27.65 psia	18 psia
Pressure drop / stage		0.1 psi	0.1 psi	0.1 psi	0.1 psi
Control variables					
Reboiler vapor		125000 lbm/hr	-	1477 lbmol/hr	97684 lbm/hr
Reboiler heat		-	3E06 Btu/hr	-	-
Top product recovery		80% A	10 lbmol/hr W	-	80% A
Btms. product recovery		-	-	95% I	-
Constraints					
Top product		$x_A \geq 95$	-	-	$x_A \geq 95$
Btms. product		$x_A \leq 25$	$x_A \leq 0.05$ $m_A \leq 25$ lbm/hr	$x_I \geq 99$	$x_A \leq 25$
Design uncertainties					
Feed flow rate	μ[a]	500 / 500	50 / 950	50 / 50	500 / 375 / 125
	σ[a]	100 / 100	10 / 10	5 / 5	12 / 25 / 30
Tray eff. (Min-Max, %)		50 - 60	30 - 40	90 - 100	50 - 70
$\lambda_{12}-\lambda_{11}/\lambda_{21}-\lambda_{22}$	μ[b]	577.47 / –234.41	–1051.1 / 1802.3	–50.331 / 76.894	577.47 / –234.41
	σ[b]	49.706 / 31.409	22.653 / 55.784	149.74 / 153.02	49.706 / 31.409
	ρ	–0.992799	–0.976212	–0.999966	–0.992799
$\lambda_{13}-\lambda_{11}/\lambda_{31}-\lambda_{33}$	μ[b]	-	-	-	751.38 / 39.546
	σ[b]	-	-	-	78.668 / 52.120
	ρ	-	-	-	–0.988954
$\lambda_{23}-\lambda_{22}/\lambda_{32}-\lambda_{33}$	μ[b]	-	-	-	–200.52 / 270.08
	σ[b]	-	-	-	28.079 / 45.828
	ρ	-	-	-	–0.999883

A = Acetone, B = Benzene, T = Toluene, M = 2-Methyl-1-Butene, I = Isoprene
μ = mean, σ = standard deviation, ρ = correlation coefficient
[a] Units are lbmol/hr
[b] Units are cal/gmol

Table 2.2. CMCI PDR evaluated with different random number set sizes.

Mixture	# Par	PDR Estimate (%)					
		100 sets	500 sets	1000 sets	2000 sets	5000 sets	10000 sets
A/B	2[a]	86	89	90	91	91	91
A/B	3[b]	74	78	81	82	82	82
A/B	5[c]	74	77	80	82	82	82
A/W	2[a]	88	92	93	94	94	94
A/W	3[b]	53	60	66	66	67	67
A/W	5[c]	54	61	66	66	67	67
M/I	2[a]	98	98	98	98	98	98
M/I	3[b]	94	95	96	96	96	96
M/I	5[c]	77	77	78	78	78	78
A/B/T	3[a]	100	100	100	100	100	100
A/ B/T	4[b]	100	99	99	100	99	99
A/B/T	10[c]	100	99	100	100	99	99

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and binary interaction parameters.

Table 2.3. CMCI PDR 95% CI length evaluated for different random number set sizes.

Mixture	# Par	95% CI					
		100 sets	500 sets	1000 sets	2000 sets	5000 sets	10000 sets
A/B	2[a]	13.6	5.5	3.8	2.5	1.6	1.1
A/B	3[b]	17.0	7.2	4.9	3.4	2.1	1.5
A/B	5[c]	17.0	7.3	4.9	3.4	2.1	1.5
A/W	2[a]	12.8	4.9	3.1	2.1	1.3	0.9
A/W	3[b]	19.2	8.5	5.9	4.2	2.6	1.8
A/W	5[c]	19.2	8.5	5.9	4.1	2.6	1.8
M/I	2[a]	6.5	2.7	1.8	1.1	0.7	0.5
M/I	3[b]	9.7	3.8	2.5	1.8	1.1	0.8
M/I	5[c]	16.3	7.3	5.1	3.6	2.3	1.6
A/B/T	3[a]	3.7	0.8	0.4	0.2	0.1	0.0
A/ B/T	4[b]	3.7	1.7	1.1	0.6	0.4	0.3
A/B/T	10[c]	3.7	1.5	1.0	0.6	0.4	0.3

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and binary interaction parameters.

2.5. Results

The OPT procedure performance is evaluated by evaluating the PDR for the case studies described in Table 2.1. The CMCI PDR estimates obtained with 10,000 sets are

used as reference to determine the accuracy of the OPT procedure. For all cases the OPT's MCI used 10,000 random sets. First it is observed the accuracy of the OPT estimates computed with only the BP's located at the axial directions from the nominal design and the MS's required. Later it is observed the additional MS's required by the OPT procedure to obtain the same PDR estimates as CMCI.

For the line-search procedure's convergence criteria, Equations 2.15 and 2.16, satisfactory results were obtained for ε_δ and ε_g equal to 1E-4. Reducing the allowed error increases the computation effort, i.e. more MS's are required to find BP's. Increasing the allowed error reduces the MS's, but reduces the accuracy of the tangent planes and hence the accuracy of the tangential estimate.

The first step size in the line-search procedure of BP's can also increase or reduce the computational effort. For the following results, with exception of the 2-methyl-1-butene / isoprene (M/I) mixture's BIP's axial directions, the first step size was set to three times the component feed flow rate's standard deviation or BIP's standard deviation or combined standard deviation, Equation 27, i.e. $M = 3$ for axial and additional BP's. For the M/I mixture's BIP's axial directions $M = 1$. This was necessary to avoid computational errors reported by the model simulation. However for additional BP's for this mixture $M = 3$ worked well. The first step in the tray efficiency's axial directions is different than for component feed flow rates and BIP's since tray efficiency's uncertainty is defined by uniform distributions. First, the tray efficiency's nominal design value is set to take the tray efficiency's maximum probable value. Then the initial step size in the positive axial direction is 0.1 times the tray efficiency's uniform distribution's length. For the negative direction, the step size is equal to the tray efficiency's uniform

distribution's length. For additional points the procedure adjusts the first step computed with Equation 27 such it does not fall outside the maximum or minimum tray efficiency's probable values.

Table 2.4 shows the initial OPT PDR estimates. These initial estimates correspond to the approximation with only the BP's at the axial directions. For eight out of the twelve cases the first tangential and optimistic PDR estimates are within one percent deviation with respect to the CMCI PDR estimates. The other four cases require few more BP's to improve the accuracy, see Table 2.5. Three out of those four cases are able to obtain estimates that are within one percent deviation with respect to the CMCI PDR estimates. For the other case, A/B mixture with five uncertain parameters, the OPT procedure is able to compute a PDR estimate that is with 1.5% deviation with respect to the CMCI PDR estimate. The twelve cases require less than 100 MS's to reach an accurate tangential PDR estimate. However, as parameter dimension increases it increases, in most of the cases, the number of MS's required to converge to an accurate PDR estimate.

On the other hand, the pessimistic approximation struggles to produce accurate PDR estimates for design cases with more than two uncertain parameters. The initial pessimistic PDR estimates have deviations of ten percent or larger with respect to the CMCI PDR estimates. The final pessimistic PDR estimates for design cases with two uncertain parameters are relatively small. However design cases with more than two uncertain parameters have final pessimistic PDR estimates with deviations larger than 20% with respect to the CMCI PDR estimates.

Table 2.4. OPT PDR estimates at initialization.

Mixture	*p*	OPT					CMCI PDR Estimate
		BP's	MS's	PDR Estimates (%)			
				Tangential	Optimistic	Pessimistic	
A/B	2[a]	4	22	90	92	82	91
A/B	3[b]	6	26	85	85	40	82
A/B	5[c]	10	42	88	88	13	82
A/W	2[a]	4	10	94	94	83	94
A/W	3[b]	6	20	67	67	30	67
A/W	5[c]	10	28	67	67	10	67
M/I	2[a]	4	16	78	97	71	98
M/I	3[b]	6	19	89	93	41	96
M/I	5[c]	10	89	78	78	1	78
A/B/T	3[a]	6	6	100	100	74	100
A/ B/T	4[b]	6	6	100	100	74	99
A/B/T	10[c]	20	20	100	100	0	99

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and binary interaction parameters.

Table 2.5. OPT PDR estimates when the tangential estimates are within 2% deviation with respect to the CMCI PDR estimates.

Mixture	*p*	OPT					CMCI PDR Estimate
		BP's	MS's	PDR Estimates (%)			
				Tangential	Optimistic	Pessimistic	
A/B	2[a]	8	38	91	91	89	91
A/B	3[b]	15	54	82	82	68	82
A/B	5[c]	24	99	83	83	31	82
A/W	2[a]	4	10	94	94	83	94
A/W	3[b]	6	20	67	67	30	67
A/W	5[c]	10	28	67	67	10	67
M/I	2[a]	9	54	98	98	94	98
M/I	3[b]	11	52	96	98	69	96
M/I	5[c]	10	89	78	78	1	78
A/B/T	3[a]	6	6	100	100	74	100
A/ B/T	4[b]	6	6	100	100	74	99
A/B/T	10[c]	20	20	100	100	0	99

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and binary interaction parameters.

Table 2.6 shows the OPT PDR estimates for the three case studies with two uncertain parameters when the convergence criterion is $\varepsilon_{OP} = 1\%$. For all three cases less than 100 MS's were required to meet the convergence criterion

Table 2.6. OPT PDR estimates for the case studies with two uncertain parameters when $\varepsilon_{OP} = 1\%$.

Mixture	p	OPT					CMCI PDR Estimate
		BP's	MS's	PDR Estimates (%)			
				Tangential	Optimistic	Pessimistic	
A/B	2[a]	10	53	91	91	90	91
A/W	2[a]	10	31	94	94	93	94
M/I	2[a]	17	81	98	98	96	98

[a] Uncertainty in feed flow rates.

Table 2.7 shows the OPT PDR estimates when 50 BP's have been used for the design cases with more than two uncertain parameters. The pessimistic estimates are not much better than those presented in Table 2.5. However the MS's increased considerably.

Table 2.7. OPT PDR estimates for designs with more than two uncertain parameters when fifty BP's are used in the CBA.

Mixture	p	OPT					CMCI PDR Estimate
		BP's	MS's	PDR Estimates (%)			
				Tangential	Optimistic	Pessimistic	
A/B	3[b]	50	213	82	82	77	82
A/B	5[c]	50	229	83	83	40	82
A/W	3[b]	50	230	67	67	31	67
A/W	5[c]	50	230	67	67	31	67
M/I	3[b]	50	295	94	96	87	96
M/I	5[c]	50	402	76	77	17	78
A/B/T	3[a]	50	50	100	100	94	100
A/ B/T	4[b]	50	112	99	99	66	99
A/B/T	10[c]	50	50	100	100	1	99

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and binary interaction parameters.

Table 2.8 presents the results obtained by the OPT tangential approximation and CMCI, including the 95% CI's for the CMCI and OPT PDR estimates. The results show

that the OPT procedures is computationally more efficient than CMCI. However, in most cases this efficiency decreases as the number of uncertain parameters increases.

Table 2.8. CMCI PDR estimates for 10,000 sets and tangential PDR estimates when the OPT procedure has added enough BP's to compute tangential estimates that are within 2% deviation with respect to the CMCI estimates.

Mixture	# Par	CMCI		Tangential		
		PDR (%)	95% CI	PDR (%)	95% CI	MS's
A/B	2[a]	91	90 - 92	91	90 – 91	38
A/B	3[b]	82	81 - 83	82	81 – 83	54
A/B	5[c]	82	81 - 83	83	82 – 84	99
A/W	2[a]	94	93 - 95	94	94 – 95	10
A/W	3[b]	67	66 - 68	67	66 – 68	20
A/W	5[c]	67	66 - 68	67	66 – 68	28
M/I	2[a]	98	98 - 98	98	98 – 98	54
M/I	3[b]	96	96 - 96	96	95 – 96	52
M/I	5[c]	78	78 - 79	78	77 – 79	89
A/B/T	3[a]	100	100 - 100	100	100 – 100	6
A/B/T	4[b]	99	99 - 100	100	100 – 100	6
A/B/T	10[c]	99	99 - 99	100	100 - 100	20

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and binary interaction parameters.

2.6. Conclusions and recommendations

The OPT procedure is shown to be two to three orders of magnitude faster than CMCI. The tangential approximation provides accurate and precise PDR estimates for a reasonable number of MS's. The tangential estimate converged accuracy is very good, usually within 1.5%.

As the number of uncertain parameters increases the advantage of the OPT procedure over CMCI is reduced. Optimization of the OPT procedures may be possible to reduce the computation effort and improve its efficiency with respect to CMCI. For more than two uncertain parameters a different convergence criterion or criteria needs to be developed.

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Chapter 3

Exploring Alternatives to Improve Procedure for Estimating Process Design Reliability (PDR)

Abstract

The certainty that a process will meet process constraints during normal operation despite the underlying uncertainty in process design parameters is the PDR. The identification of unnecessarily oversized or critically undersized equipment by PDR estimation and sensitivity analysis leads to better safety factor selection and more importantly to ensure capital investment. A major limitation to estimate PDR is computational cost. This chapter presents analysis and modifications to improve the procedure to estimate PDR by geometrically mapping the constraint boundary coupled with Monte Carlo integration. Example problems discussed include multicomponent distillation and geometrical cases.

3.1. Introduction

Process design reliability has been traditionally estimated by conventional Monte Carlo integration (CMCI). CMCI is computationally too expensive since it requires a large number of model simulations (MS's) to converge to an acceptable estimate (see Chapter 2). An alternative developed at the Kurata Thermodynamics Laboratory is the optimistic-pessimistic-tangential (OPT) procedure, i.e. Monte Carlo integration (MCI) of the *c*-constraints mapped onto the *p*-parameter space (MacDonald, 1993; Howat, 1995). The fundamental difference between CMCI and the OPT procedure is that the OPT procedure separates the process simulations from the MCI statistics. The OPT

methodology geometrically interpolates among constraint boundary points to determine the fraction of parameter sets that fall within the interpolated boundary. Confidence in the reliability estimate is improved with increasing number of boundary points (BP's). Results presented in Chapter 2 show that the OPT method is computationally more efficient than CMCI. However, as the number of BP's required to approximate the constraint boundary (CB) increases, the advantage of the OPT method over CMCI decreases.

Consider the case study presented in Chapter 2 which is a distillation column to separate an acetone/benzene (A/B) mixture with the component feed flow rates as the uncertain parameters. The OPT procedure initiates the PDR estimation by finding the BP's located at the axial directions of the nominal design. These BP's, determined using only a few MS's, are used to compute tangent and connecting planes that make up three constraint boundary approximations (CBA's). The CBA's serve to evaluate three PDR estimates by MCI: tangential (TPDR), optimistic (OPDR) and pessimistic (PPDR) PDR estimates. Table 3.1 shows the number of MS's required at this first iteration, i.e. initialization. The difference between the optimistic and the pessimistic estimates define the uncertainty in the estimates. Table 3.1 also includes the PDR estimate evaluated by CMCI. The initial TPDR and CMCI PDR estimates are the same indicating that the tangential boundary interpolation is generally adequate with few MS's. Because of the significant difference between the OPDR and PPDR estimates, one or more additional BP's are required to determine whether the initial TPDR estimate is sufficiently accurate.

The procedure determines the direction in the parameter space to search for a new BP based on the MCI statistics and the current subdivision of the parameter. At initialization

Table 3.1. Results of the OPT procedure at initialization for the A/B case study with two uncertain parameters (feed flow rates).

Mixture	*p*	OPT (MCI with 10,000 sets)						CMCI[a] PDR (%)
		BP's	NNG's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	
A / B	2	4	4	25	91	92	82	91
[a] CMCI with 10,000 MC sets								

the OPT procedure divides the parameter space in 2^p nearest-neighbor groups (NNG's). The MCI procedure keeps track of the number of parameter sets that fall inside each NNG and inside each of the NNG CBA's. The search for a new BP is conducted in the direction of the NNG with the largest uncertainty, i.e. the NNG with the largest number of parameter sets that fall inside the optimistic CBA, but outside the pessimistic CBA. Each time a new BP is added, the procedure destroys the NNG where the new BP falls and creates *p* new NNG's. The addition of BP's continues until the difference between the optimistic and pessimistic estimates is not significant. Table 3.2 shows for the acetone/benzene case that adding at least one more BP to each of the initial NNG's serves to improve the OPDR and PPDR estimates and verify the accuracy of the TPDR estimate. Nonetheless, adding four BP's doubles the number of MS's. This case requires few initial and final MS's with respect to CMCI. However, for cases with a larger number of uncertain parameters or more complicated CB's, the MS's increase rapidly, i.e. the efficiency of the OPT procedures is compromised.

This chapter analyzes options to improve the efficiency in estimating PDR by CBA coupled with MCI. The modified methodology is tested with multicomponent distillation and geometrical case studies.

Table 3.2. Summary of MCI statistics as new BP's are added by the OPT procedure for the A/B case study with two uncertain parameters.

BP's	NNG's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	BP Added to NNG
4	4	25	91	92	82	-
5	5	26	91	92	86	4
6	6	35	90	91	87	2
7	7	36	90	91	88	3
8	8	44	91	91	89	1

3.2. Problem definition and proposed modification

The OPT procedure employs MS's to search for BP's and for evaluating partial derivatives using finite differences. The BP's are used to construct the CBA's using connecting and tangent planes. The partial derivatives at each BP are required to compute tangent planes. The total MS's required by the OPT procedure to estimate the PDR of a process design with p uncertain parameters may be computed by:

$$S = \sum_{i=1}^{N^{BP}} s_i + N^{BP} p \tag{3.1}$$

where s_i is the MS's required to find the i-th BP and N^{BP} is the number of BP's. $N^{BP} p$ corresponds to the MS's required to evaluate the derivatives.

The OPT procedure initializes the CBA's by using only the $2p$ BP's located at the axial directions from the nominal design. Expanding Equation 3.1 to separate the MS's required for initializing from those required for improving or verifying the accuracy of the CBA, it results in:

$$S = \sum_{i=1}^{2p} s_i + 2p^2 + \sum_{i=2p+1}^{N^{BP}} s_i + (N^{BP} - 2p)p \tag{3.2}$$

The first two terms in the right side of Equation 3.2 correspond to the MS's required at initialization. The number of BP's required to approximate with sufficient accuracy the

CB of any given design case depends on its specific geometry and is commonly unknown in advance. When at least one more BP inside each of the 2^p initial NNG's is necessary to accurately approximate the CB, the MS's required may be computed by:

$$S = \sum_{i=1}^{2p} s_i + 2p^2 + \sum_{i=2p+1}^{2p+2^p} s_i + 2^p p \tag{3.3}$$

The number of NNG's resulting is $p\ 2^p$. Adding a new BP inside each of these NNG's will result in $p^2\ 2^p$ NNG's. Defining A as the required number of times that new BP's need to be added to the existing NNG's, $p^A\ 2^p$ NNG's will result. The expression for computing the MS's is:

$$S = \sum_{i=1}^{2p} s_i + 2p^2 + \sum_{i=2p+1}^{2p+\sum_{j=1}^{A} p^{j-1} 2^p} s_i + p \sum_{j=1}^{A} p^{j-1} 2^p \tag{3.4}$$

This equation shows that the MS's required for computing the partial derivatives at each BP makes the total MS's increase very rapidly.

However, if only connecting planes were used to approximate the CB, the MS's may be computed by:

$$S = \sum_{i=1}^{2p} s_i + \sum_{i=2p+1}^{2p+\sum_{j=1}^{A} p^{j-1} 2^p} s_i \tag{3.5}$$

This equation shows that the MS's may be reduced by eliminating the tangential planes computations. This chapter tests the alternative of eliminating the use of tangent planes and only using connecting planes to approximate the CB. It includes improvements in the procedure to improve the CBA by connecting planes and to reduce MS's required to find BP's.

3.3. Modified procedure development

In the following sections the modified procedure is referred to as the statistically most significant direction (SMSD) procedure. Because only connecting planes are used to approximate the CB, the SMSD procedure computes only one type of CBA so for a given number of BP's only one PDR estimate is evaluated by MCI. Consequently new methodologies were developed to determine the search direction for new BP's and to determine the convergence. The main steps of the SMSD procedure are outlined in the flow chart presented in Figure 3.1 and described below.

The SMSD procedure starts the CBA in the same way as the OPT does, with the BP's located at the 2p axial direction from the nominal design. The BP's are found using the line-search procedure described in Section 2.3.2 with a few modifications:

a. The initial step size for the initial 2p BP's is set to four times the standard deviation of the uncertain parameter in turn, i.e. $M = 4$, with exception of the tray efficiency axial direction, where it follows the same procedure as described in Section 2.5. The valor of four is used to reduce underestimation in CB's located close to the farthest significant distance. For the BP's that are added later $M = 3$ to reduce the MS's that the line-search procedure may require.

b. Section 2.3.2 describes the use of the Regula-Falsi method and a methodology to speed up the convergence when the procedure may be "stuck" in one region of the search interval. This methodology tests if the new bracketing value, δ, is too close to the previous low (δ_{low}) or high (δ_{high}) bracketing value. If that is the case, the methodology re-computes the bracketing value in the following way:

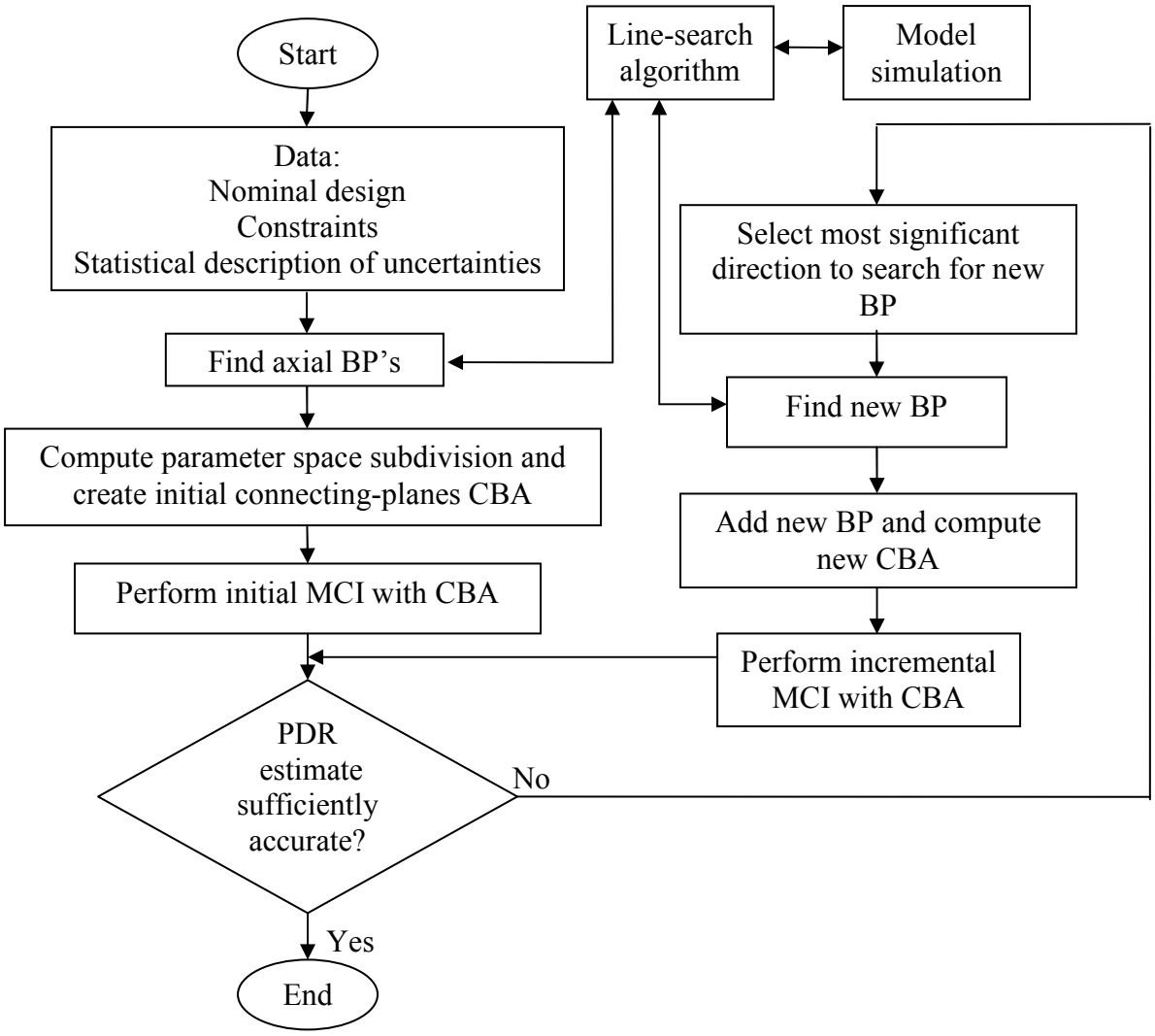


Figure 3.1. SMSD procedure to estimate PDR.

$$\delta = \delta_{low} + 1.5 \times \left(\delta - \delta_{low}\right) \text{ if } \frac{\delta - \delta_{low}}{\delta_{high} - \delta_{low}} \leq 0.30 \tag{3.6}$$

$$\delta = \delta_{high} - 1.5 \times \left(\delta_{high} - \delta\right) \text{ if } \frac{\delta_{high} - \delta}{\delta_{high} - \delta_{low}} \leq 0.30 \tag{3.7}$$

However the constraints in Equations 3.6 and 3.7 may also be true for cases when the method is not really "stuck". In such cases the methodology actually slows the convergence. Therefore, the methodology was modified such that the bracketing

value is recomputed only if in two subsequent iterations the new bracketing value is too close to one of the previous δ_{low} or δ_{high} .

c. The convergence criteria for the line-search procedure is given by the following equations:

$$\delta_{high} - \delta_{low} < \varepsilon_{\delta} \tag{3.8}$$

$$\left| \underset{i=1,\ldots,c}{Max}\{g_i\} \right| < \varepsilon_g \tag{3.9}$$

For the OPT procedure accurate computations of BP's and constraints values are required since they are used to compute partial derivatives by finite differences that are later used to compute the tangent planes. For the SMSD procedure the convergence criteria can be relaxed to reduce the MS's without affecting the accuracy of the MCI.

After the 2*p* initial BP's have been found, the procedure divides the parameter space in 2^p NNGs using Equation 2.10. Later, the procedure computes the connecting planes that make up the initial CBA using Equations 2.17 and 2.18.

For the MCI, the SMSD generates the MC sets as described in Chapter 2. As each MC set is generated, it is examined to find the NNG in which it resides and to determine if the set falls inside or outside the NNG's CBA using Equations 2.18 and 2.21. If a NNG has only non-failure BP's, the procedure does not use the connecting plane CBA for that NNG and instead it assumes that all the MC sets that fall in that NNG are inside the CB. This assumption speeds up the convergence avoiding unnecessary computations and works well for the case studies of this work, which are open-ended in some regions of the parameter space. The MCI procedure keeps track of the number of sets that resides

in each NNG, N_i^T, and the number of sets for each NNG that fall outside the boundary approximation F_i. The SMSD PDR estimate, $\hat{\Re}^{SMSD}$, is computed as a percentage:

$$\hat{\Re}^{SMSD} = 100N^{-1}\sum_{i=1}^{N^N}\left(N_i^T - F_i\right) \tag{3.10}$$

In this equation N^N is the number of NNG's and N is the number of MC sets.

A new metric based on the statistically most significant direction is incorporated into the procedure to select the direction to search for an additional BP to improve the CBA. First a centered location of the MC sets that fall outside each NNG's CBA is computed:

$$\theta_{k,j}^a = \frac{\sum_{i=1}^{N_k^{SO}}\theta_{i,j}}{N_k^{SO}}, \quad j = 1,2,..,p \tag{3.11}$$

Here N_k^{SO} is the number of sets outside the k-th NNG's boundary approximation. Then a dimensionless distance is computed. If the NNG has no non-failure points the following equation is used:

$$d_k = \frac{\sqrt{\sum_{j=1}^{p}\frac{\left(\theta_{k,j}^a - \theta_j^D\right)^2}{\tau_j}}}{\left(100 \cdot N_k^{SO}/N\right)} \tag{3.12a}$$

If the NNG has any non-failure points the distance is computed by:

$$d_k = \frac{\sqrt{\sum_{j=1}^{p}\frac{\left(\theta_{k,j}^a - \theta_j^D\right)^2}{\tau_j}}}{\left(100 \cdot \left(N_k^{SO}\right)^2/N\right)} \tag{3.12b}$$

In these equations θ_j^D is the *j*-th coordinate of the nominal design and τ_j is a factor to dimensionless the *j*-th parameter. For a parameter with uncertainty defined by a normal distribution, the factor is given by:

$$\tau_j = 4\sigma_j \tag{3.13a}$$

For a parameter which uncertainty is defined with a uniform distribution the factor is computed by:

$$\tau_j = \theta_j^{MAX} - \theta_j^{MIN} \tag{3.13b}$$

The NNG with the most significant direction is the NNG that has the shortest computed dimensionless distance. A radial vector $\vec{r}$ pointing at the same direction as the most significant direction is computed using the centered location of the MC sets that fall outside the NNG and Equation 2.25.

The SMSD procedure adds iteratively new BP's to improve the PDR estimate. The procedure uses the MCI results to evaluate the convergence of each NNG. When all NNG's have reached convergence the procedure stops adding BP's and the calculations end. The convergence criteria for each NNG follow:

1. When a NNG has only non-failure BP's, it is assumed that all the NNG's statistical significant parameter space is inside the CB and no further computations are required for that NNG.
2. When a new BP is found in the *i*-th NNG, *p* new NNG's are created. The procedure keeps track of the number of MC sets that fell outside the CBA of the old *i*-th NNG, F_i^{old}, and the number of MC sets that fall outside the new *p* NNG's: F_i^{new},

$F_{N^N-p+2},\ldots,F_{N^N}$. The p new NNG's have reached convergence if the percentage of change in the number of sets that fell outside the CBA is relatively small, i.e:

$$\frac{\left|F_i^{old}-\left(F_i^{new}+\sum_{k=N^N-p+2}^{N^N}F_k\right)\right|}{F_i^{old}}\times 100 < c_1 \tag{3.14}$$

or

$$\frac{\left|F_i^{old}-\left(F_i^{new}+\sum_{k=N^N-p+2}^{N^N}F_k\right)\right|}{N^{MC}}\times 100 < c_2 \tag{3.15}$$

3.4. Case studies, results and discussion

To evaluate the procedure several geometrical and distillation column design examples are considered. The first four case studies are geometrical cases with two uncertain parameters. Two cases have open-ended constraint boundaries with similar shapes to two of the distillation column designs. The other two cases have closed constraint boundaries. The distillation column design case studies considered are the same as those presented in Table 2.1.

The procedure is evaluated by comparing its performance to the OPT performance. The two procedures use the same number of MC sets (10,000) for the geometrical and distillation case studies.

For the geometrical cases the OPT procedure uses $\varepsilon_\delta = 1E-4$ and $\varepsilon_g = 1E-4$ for the line-search's convergence criteria, Equations 2.15 and 2.16 in Chapter 2. For the search of axial BP's and additional points $M = 3$. Because the four geometrical case studies have only two uncertain parameters, the OPT procedure convergence criterion is defined

by Equation 2.28 with $\varepsilon_{OP} = 1\%$. The SMSD procedure uses $\varepsilon_{\delta} = 1E-2$ and $\varepsilon_{g} = 1E-2$ for the line-search's convergence criteria. As defined in Section 3.3, the SMSD procedure uses $M = 4$ for the search of axial BP's and $M = 3$ for the search of additional BP's. The SMSD procedure's convergence criteria is $c_1 = 10.0\%$ and $c_2 = 0.7\%$.

The first geometrical case study has a CB similar to the A/B distillation column with the two component feed flow rates being the uncertain parameters. The second case has a CB similar to the 2-methyl-1-butene/isoprene (M/I) and the acetone/water (A/W) distillation columns with the two component feed flow rates being the uncertain parameters. Parameter uncertainties are described by normal distributions. The CB equations and uncertainty statistical descriptions for both cases are given in Table 3.3. Figures 3.2 and 3.3 show the CB's in the parameter space for the first and second case studies respectively.

Table 3.3. CB equations and statistical description of parameter uncertainty for the first and second case studies.

Case study	Nominal design (θ_1, θ_2)	Parameter uncertainty	Constraint boundary equations
First	500, 500	θ_1 is N(500, 100) θ_2 is N(500, 100)	$g_1 = \theta_2 - \frac{1}{460}(\theta_1 - 950)^2 - 400 \le 0$ $g_2 = \frac{48}{75}(\theta_1 - 500) + 308 - \theta_2 \le 0$
Second	50, 50	θ_1 is N(50, 5) θ_2 is N(50, 5)	$g_1 = \theta_1 + \frac{1}{120}(\theta_2 - 52)^2 - 61 \le 0$
N(μ,σ) = Normal distribution with mean μ and standard deviation σ.			

Tables 3.4 and 3.5 present the results from the OPT, SMSD and CMCI procedures for the first and second case studies. The results presented correspond to the initial estimates with the axial BP's and added BP's until the procedures have met their convergence

criterion or criteria. For the first case study the SMSD procedure requires 50% of the MS's that the OPT procedure requires to reach the CMCI PDR estimate. Furthermore the SMSD procedure requires fewer MS's to determine that all the NNG's have met the convergence criteria than the OPT requires to meet its convergence criterion.

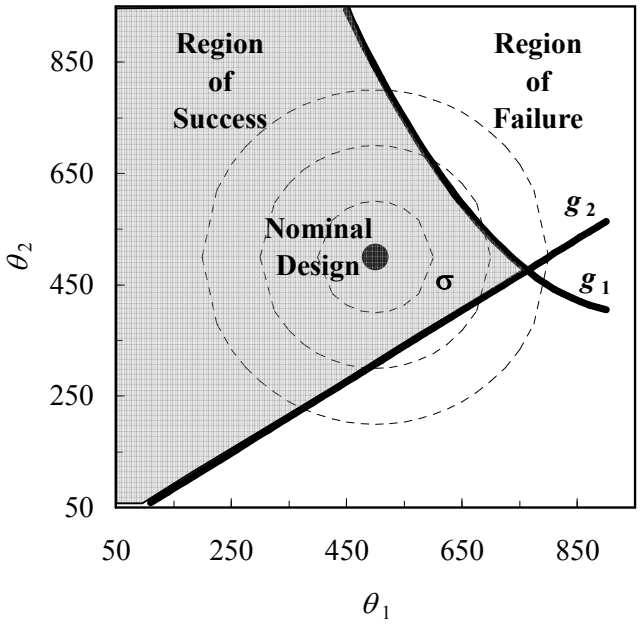


Figure 3.2. CB in parameter space for first geometrical case study.

For the second case study, the SMSD procedure requires 36% of the MS's the OPT procedure requires to reach the CMCI PDR estimate. However for this case the SMSD procedure requires few more MS's to determine that all the NNG's have met the convergence criteria than the OPT requires to meet its convergence criterion. Nevertheless the SMSD procedure estimate reaches the CMCI PDR estimate faster than the OPT pessimistic approximation does. This can be better observed in Figure 3.4.

For the first and second case studies the SMSD procedure requires approximately the same number of BP's as the OPT procedure to reach the CMCI PDR estimate, however

in both cases, independently of the MS's, the SMSD procedure requires more BP's to meet the convergence criteria.

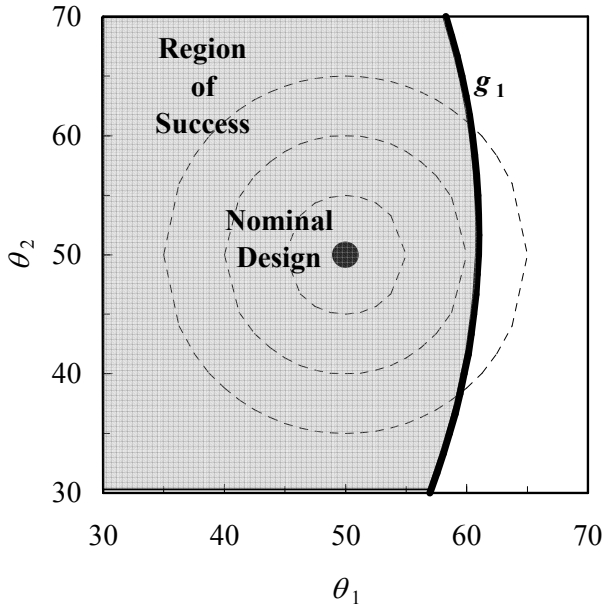


Figure 3.3. CB in parameter space for second geometrical case study.

Table 3.4. First case study PDR estimates evaluated by the OPT and SMSD procedures. CMCI PDR estimate with 10,000 MC sets is 92%.

	OPT				SMSD	
BP's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	MS's	PDR (%)
4	17	90	92	82	12	87
5	18	90	92	87	13	90
6	25	91	92	88	16	90
7	26	91	92	89	17	91
8	32	91	92	91	21	92
9	40	92	92	91	24	92
10					27	92
11					32	91

Table 3.5. Second case study PDR estimates evaluated by OPT and SMSD procedures. CMCI PDR estimate with 10,000 MC sets is 98%.

	OPT				SMSD	
BP's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	MS's	PDR (%)
4	8	99	99	90	6	95
5	15	99	99	92	10	96
6	22	98	98	94	14	98
7	23	98	98	96	18	98
8	24	98	98	97	21	98
9	25	98	98	98	25	98
10					28	98

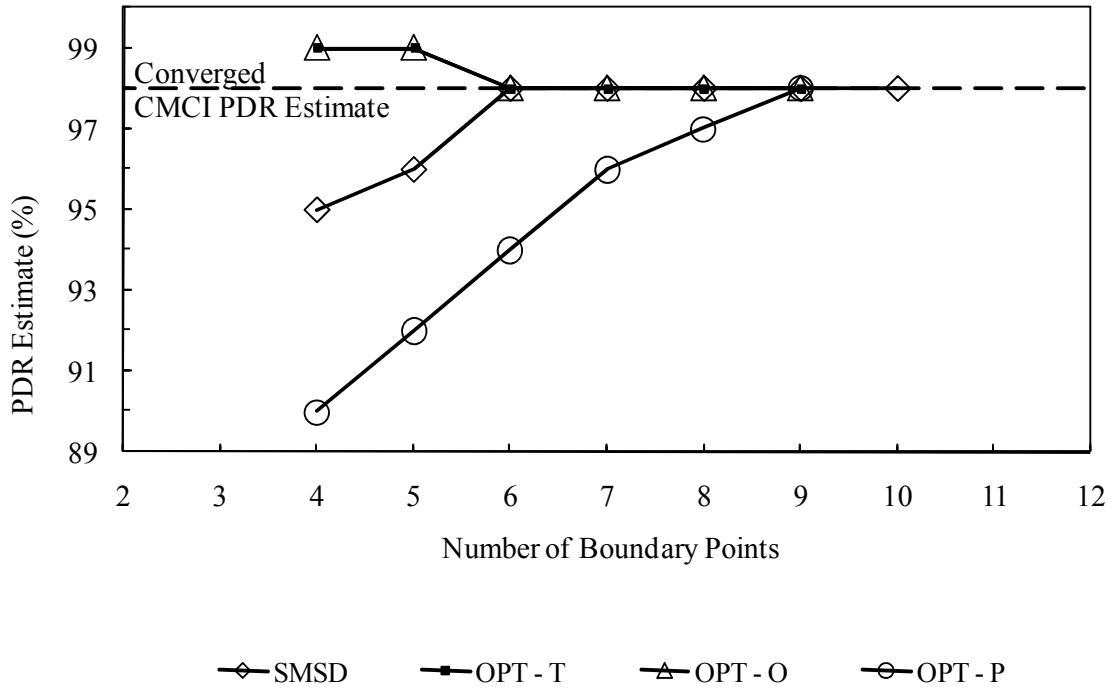


Figure 3.4. PDR estimate as a function of the number of BP's estimated for the second geometrical case study.

The third and fourth case studies were designed to observe how the CB shape affects the SMSD procedure's performance. The CB's in the parameter space for these case studies are shown in Figures 3.5 and 3.6.

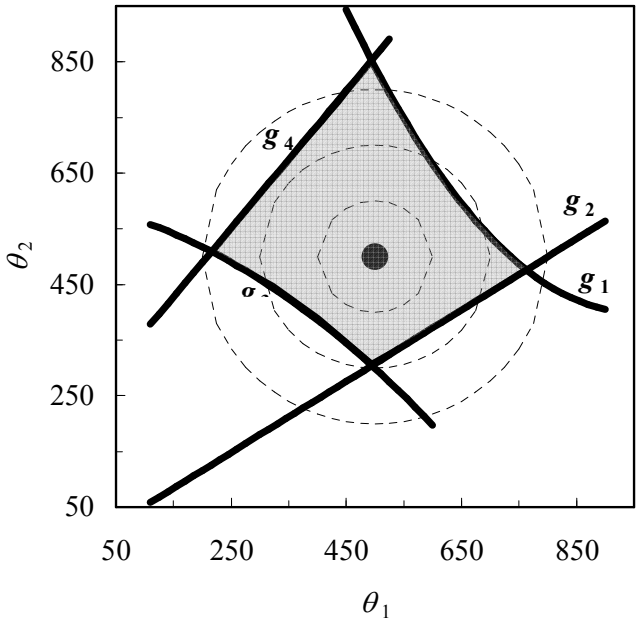


Figure 3.5. CB in parameter space for third geometrical case.

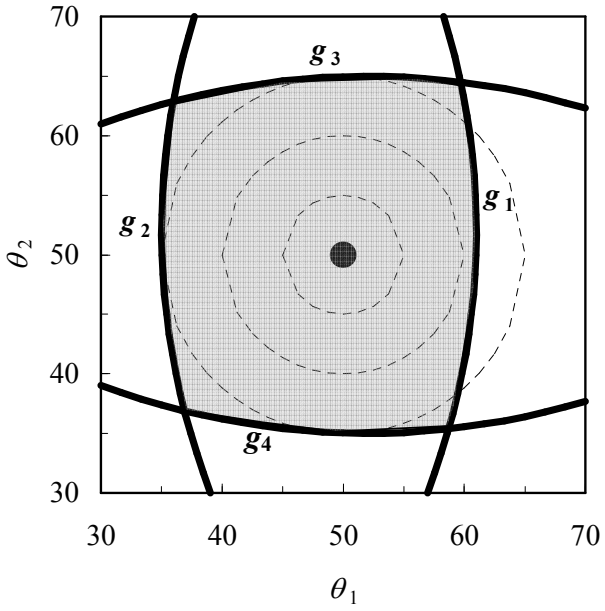


Figure 3.6. CB in parameter space for fourth geometrical case study.

Table 3.6 presents the CB equations and the parameter uncertainty statistical descriptions for both cases. Table 3.7 and 3.8 present the evaluation results for the third and fourth case studies respectively. For the third case study, the SMSD procedure requires 57% of the MS's the OPT procedure requires to reach the CMCI PDRE. Also for this case the SMSD procedure requires less MS's to determine that all the NNG's have met the convergence criteria than the OPT requires to meet its convergence criterion. However for the fourth case the SMSD requires almost double the MS's than the OPT requires to reach the CMCI PDR estimate. In spite of that, the SMSD requires the same MS's to determine that all the NNG's have met the convergence criteria than the OPT requires to meet its convergence criterion. For the third case study the SMSD requires only one more BP than the OPT procedure does. However for the fourth case, the SMSD procedure requires double the number of BP's than the OPT procedure does.

The results of the first three case studies show that the SMSD procedure can obtain accurate PDR estimates with fewer MS's than the OPT procedure does. However the SMSD procedure requires more BP's to meet the convergence criteria. This is because in order to verify the accuracy of the estimate, the procedure must check the CBA for each initial or new NNG by checking that the addition of a BP to the NNG does not considerably change the PDR estimate.

The results of the last two case studies show that the design CB shape and the ability of one procedure to approximate it with the less possible number of BP's are critical factors in the advantage of one method over the other. For the third case study, the initial SMSD procedure's CBA has a diamond shape that is fairly close to the actual CB and sets the opportunity for the advantage of the SMSD procedure over the OPT procedure.

For the fourth case study, the initial OPT procedure's tangential CBA has a quadrilateral shape that is closer to the actual CB than the SMSD procedure's diamond shaped CBA is.

Table 3.6. CB equations and statistical description of parameter uncertainty for the third and fourth case studies.

Case study	Nominal design (θ_1, θ_2)	Parameter uncertainty	Constraint boundary equations
Third	500, 500	θ_1 is N(500, 100) θ_2 is N(500, 100)	$g_1 = \theta_2 - \frac{1}{460}(\theta_1 - 950)^2 - 400 \le 0$ $g_2 = \frac{48}{75}(\theta_1 - 500) + 308 - \theta_2 \le 0$ $g_3 = -\theta_2 - \frac{1}{1400}(\theta_1 + 160)^2 + 610 \le 0$ $g_4 = \theta_2 - \frac{21}{17}(\theta_1 - 500) + 860 \le 0$
Fourth	50, 50	θ_1 is N(50, 5) θ_2 is N(50, 5)	$g_1 = \theta_1 + \frac{1}{120}(\theta_2 - 52)^2 - 61 \le 0$ $g_2 = -\theta_1 + \frac{1}{120}(\theta_2 - 52)^2 + 35 \le 0$ $g_3 = \theta_2 + \frac{1}{120}(\theta_1 - 52)^2 - 65 \le 0$ $g_3 = -\theta_2 + \frac{1}{120}(\theta_1 - 52)^2 + 35 \le 0$
N(μ,σ) = Normal distribution with mean μ and standard deviation σ.			

Table 3.7. PDR estimates for third case study evaluated by OPT and SMSD procedures. CMCI PDR estimate with 10,000 MC sets is 85%.

	OPT				SMSD	
BP's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	MS's	PDR (%)
4	25	82	87	79	16	84
5	33	84	87	81	20	85
6	39	83	86	81	25	85
7	46	85	85	83	28	85
8	52	85	85	84	31	85
9	60	85	85	84	36	84
10					39	85

Table 3.8. PDR estimates for fourth case study evaluated by OPT and SMSD procedures. CMCI PDR estimate with 10,000 MC sets is 98%.

	OPT				SMSD	
BP's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	MS's	PDR (%)
4	23	98	98	90	12	90
5	30	98	98	92	16	92
6	37	98	98	94	20	94
7	45	98	98	96	24	96
8	53	98	98	97	28	97
9					32	97
10					35	97
11					38	97
12					41	98
13					44	98
14					47	98
15					50	98
16					53	98

The distillation case studies' specifications are presented in Table 2.1. The OPT procedure's line-search convergence criteria and initial step sizes are the same as those described in Section 2.5. For designs with two uncertain parameters the procedure uses the convergence criterion defined by Equation 2.28 with $\varepsilon_{OP} = 1\%$.

The SMSD procedure uses $\varepsilon_{\delta} = 1E-3$ and $\varepsilon_{g} = 1E-3$ for the modified line-search's convergence criteria procedure, described in the previous section. With exception of the A/B and M/I designs, the SMSD procedure uses $M = 4$ for the search of axial BP's as defined in Section 3.3. For the A/B designs the initial step in the feed flow rate negative axial direction with respect to the nominal design was $M = 3$. This was necessary because when using $M = 4$ the distillation model simulator was unable to converge. For the M/I design with five uncertain parameters, the search of axial BP's in the BIP's directions uses $M = 1$ so the model simulator converges. For the search of additional points, the SMSD procedure uses $M = 3$ as defined in Section 3.3. The SMSD procedure

uses c_1 = 10.0%, c_2 = 1.0% for the convergence criteria as defined by Equation 3.14 and 3.15.

Tables 3.9, 3.10 and 3.11 show the progress of the OPT and SMSD procedures as BP's are added to the CBA for the design cases with two uncertain parameters. For the A/B and A/W designs, the initial OPT tangential PDR estimates are more accurate than the SMSD PDR estimates.

Table 3.9. PDR estimates for the A/B distillation column with two uncertain parameters (feed flow rates) evaluated by the OPT and SMSD procedures. CMCI PDR estimate with 10,000 MC sets is 91%.

	OPT				SMSD	
BP's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	MS's	PDR (%)
4	22	90	92	82	14	85
5	23	90	92	86	15	89
6	30	90	91	87	16	90
7	31	90	91	88	22	90
8	38	91	91	89	26	91
9	46	91	91	90	29	91
10	53	91	91	90		

Table 3.10. PDR estimates for the A/W distillation column with two uncertain parameters (feed flow rates) evaluated by the OPT and SMSD procedures. CMCI PDR estimate with 10,000 MC sets is 94%.

	OPT				SMSD	
BP's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	MS's	PDR (%)
4	10	94	94	83	9	89
5	19	94	94	87	14	91
6	27	94	94	90	21	93
7	28	94	94	91	26	93
8	29	94	94	92	31	94
9	30	94	94	93	36	94
10	31	94	94	93	41	94

For the A/B design the two procedures require the same number of BP's to reach the CMCI PDR estimate. However the SMSD procedure requires fewer MS's to reach the CMCI PDR estimate and to meet its convergence criteria than the OPT procedure does. These results agree with the findings for the first geometrical case study.

Table 3.11. PDR estimates for the M/I distillation column with two uncertain parameters (feed flow rates) evaluated by the OPT and SMSD procedures. CMCI PDR estimate with 10,000 MC sets is 98%.

	OPT				SMSD	
BP's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	MS's	PDR (%)
4	16	78	97	71	16	94
5	17	89	99	82	22	96
6	26	94	99	87	27	97
7	37	97	99	90	28	98
8	46	96	98	92	29	98
9	54	98	98	94	35	98
10	55	98	98	95	41	98
11	56	98	98	96	47	98
12	67	97	98	96	53	98
13	68	97	98	96		
14	69	97	98	96		
15	70	97	98	96		
16	71	97	98	96		
17	81	98	98	96		

For the A/W design the OPT procedure has advantage over the SMSD procedure because of the CB shape. The SMSD procedure requires more BP's to approximate accurately the CB and to meet the convergence criteria than the OPT procedure does. These results agree with the findings for the second geometrical case study. However the two procedures use the same BP's because the OPT pessimistic approximate requires more BP's to reach an accurate PDR estimate than the SMSD procedure does.

For the M/I design an initial error of 20% in the OPT tangential PDR estimate does not agree with the results for the second geometrical case study and the A/W design with

two uncertain parameters. Because of this, the SMSD procedure is able to compute a more accurate PDR estimate with fewer MS's than the OPT procedure, even though they use the same BP's.

The problem in the OPT tangential PDR estimate is caused by an inability of the line-search procedure and model simulator to converge to an accurate axial BP for this design. It is observed that when the OPT procedure uses a different initial step size in the search of the axial BP, the line-search procedure converges to a slightly different BP. Figure 3.7 shows the constraint value as a function of the 2-methyl-1-butene feed flow rate for the nominal design isoprene feed flow rate. This graph also includes the computed BP's when using for the initial step sizes $M = 3$ and $M = 4$. This figure shows the errors in the two computed BP's.

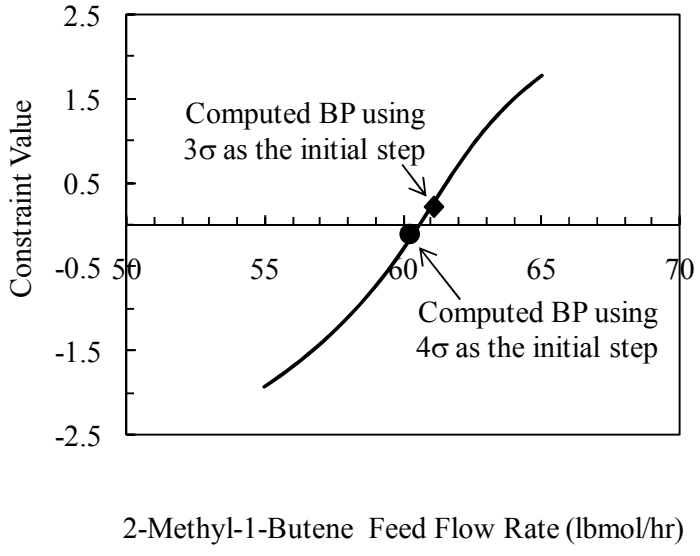


Figure 3.7. M/I design constraint value as a function of the 2-methyl-1-butene feed flow rate for the nominal design isoprene feed flow rate. BP's found when using initial step sizes of three and four times the 2-methyl-1-butene feed flow rate's standard deviation.

Despite the error in the BP when using four times the standard deviation, the initial OPT tangential PDR estimate is more accurate, see Table 3.12. What happens here is that the procedure is able to determine that the computed tangent plane is incorrect. The procedure does this by checking the position of the nominal design with respect to the tangent plane. Then the procedure replaces the incorrect tangent plane by the orthogonal plane to the computed BP. Figures 3.8 and 3.9 show the computed BP's and tangents in the feed components parameter space. The included CMCI results define the design's CB shape and allow seeing the error in the tangent planes. Figure 3.9 includes the orthogonal plane to the computed BP. Because the orthogonal plane is close to the actual tangent, the tangential PDR estimate is accurate. When using the initial step size of three times the flow rate's standard deviation the OPT procedure is not able to detect that the computed tangent plane is incorrect and produces a large error in the initial tangential PDR estimate.

Table 3.12. OPT and SMSD PDR estimates for the M/I distillation column with two uncertain parameters. An initial step for search of axial BP's of four times the standard deviation is also used for the OPT procedure.

	OPT				SMSD	
BP's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	MS's	PDR (%)
4	23	98	98	94	16	94
5	33	98	98	95	22	96
6	41	97	98	97	27	97
7	42	97	98	97	28	98
8	43	98	98	97	29	98
9					35	98
10					41	98
11					47	98
12					53	98

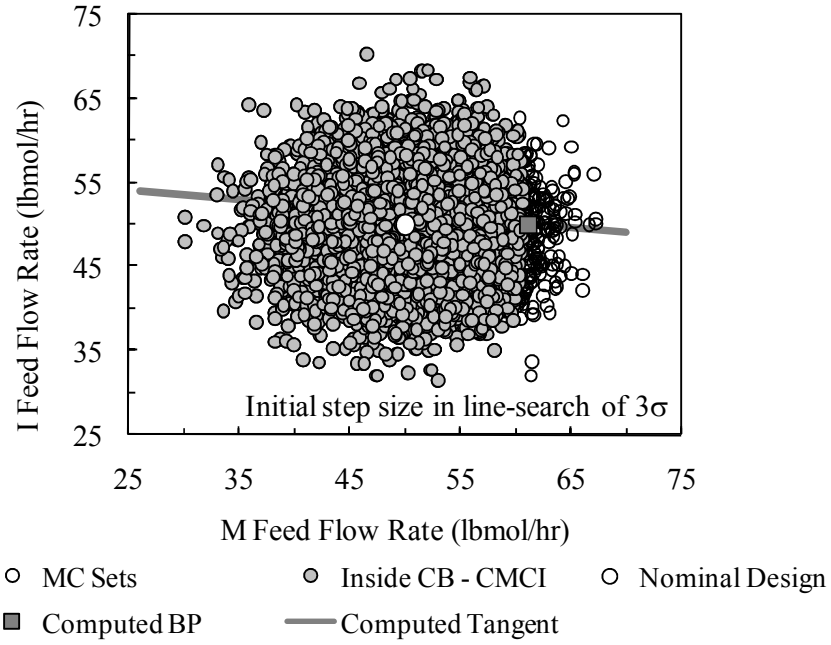


Figure 3.8. CMCI results in the parameter space for the M/I design with two uncertain parameters. The graph shows the axial BP and its tangent when using $M = 3$.

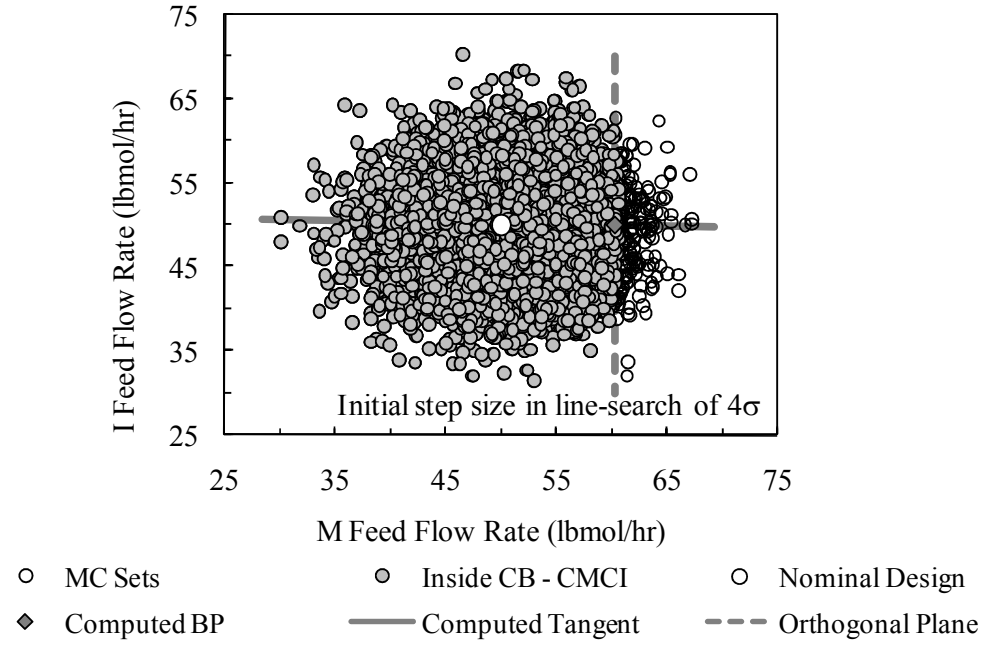


Figure 3.9. CMCI results in the parameter space for M/I design with two uncertain parameters. The graph shows the axial BP found when using $M = 4$ and the orthogonal plane used by the OPT procedure to replace the incorrect tangent.

Table 3.13 presents the OPT and SMSD PDR estimates computed with only the axial BP's for the distillation case studies with more than two uncertain parameters. The M/I design with three uncertain parameters includes OPT estimates when using $M = 4$ for the initial step size. The A/B/T case with ten uncertain parameters includes the SMSD estimate when $M = 3$ for the initial step size in the search of BIP's axial BP's. Doing this makes the SMSD procedure find only non-failure BP's. So rather than using connecting planes to approximate the CB, the procedure assumes all the MC sets fall inside the successful space. This produces an error of 1% in the SMSD PDR estimate with respect to the CMCI PDR estimate. With the exception of the ternary mixture case studies, for all the case studies with more than two uncertain parameters the SMSD procedure considerably underestimates the PDR. This is because, with the exception of the A/B/T designs, for designs with more than two uncertain parameters the axial BP's are not enough for the SMSD procedure to make an accurate approximation of the CB. The problem increases as dimension increases.

Table 3.14 shows the SMSD PDR estimates when the procedure has met the NNG's convergence criteria and the OPT PDR estimates when the tangential estimate is within 2% error with respect the CMCI PDRE. The results for the cases with more than two uncertain parameters show that the SMSD procedure is unable to approximate accurately their CB's. The ternary mixture cases are an exception because the SMSD procedure finds only non-failure BP's and uses the NNG's convergence criterion for NNG's with only non-failure BP's rather than using connecting planes to approximate the CB. For designs with more than two uncertain parameters the tangential OPT PDR estimate provides the most accurate result with the lowest computational effort. However the

pessimistic OPT PDR estimate underestimates considerably the PDR for design with more than two uncertain parameters. The convergence criterion based on the optimistic and pessimistic estimates cannot be used. CMCI PDR estimates are not normally known a priori. Therefore for designs with more than two uncertain parameters the OPT procedure requires an efficient way to evaluate when convergence to an accurate PDR estimate has been reached.

Table 3.13. Initial PDR estimates for OPT and SMSD procedures.

Mixture	p	BP's	OPT				SMSD		CMCI PDR (%)
			MS's	TPDR (%)	OPDR (%)	PPDR (%)	MS's	PDR (%)	
A/B	3[b]	6	26	85	85	40	16	42	82
A/B	5[c]	10	42	88	88	13	24	16	82
A/W	3[b]	6	20	67	67	30	15	36	67
A/W	5[c]	10	28	67	67	10	19	17	67
M/I	3[b]	6	19	89	93	41	18	72	96
M/I[d]	3[b]	6	26	98	98	53	-	-	-
M/I	5[c]	10	89	78	78	1	54	1	78
A/B/T	3[a]	6	6	100	100	74	6	100	100
A/ B/T	4[b]	8	6	100	100	74	8	100	99
A/B/T	10[c]	20	20	100	100	0	24	3	99
A/B/T[e]	10[c]	20	-	-	-	-	20	100	-

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and binary interaction parameters (BIP's).
[d] For line search of axial BP's $M = 4$ for the component feed flow rate.
[e] For line search of axial BP's $M = 3$ for the BIP's.

Table 3.14. SMSD PDR estimates when the method has met the convergence criteria for designs with more than two uncertain parameters. OPT PDR estimates when the tangential estimates are within 2% deviation with respect to the CMCI PDR estimates.

Mixture	p	OPT					SMSD			CMCI PDR (%)
		BP's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	BP's	MS's	PDR (%)	
A/B	3[b]	15	54	82	82	68	31	73	76	82
A/B	5[c]	24	99	83	83	31	56	116	42	82
A/W	3[b]	6	20	67	67	30	25	63	59	67
A/W	5[c]	10	28	67	67	10	46	118	38	67
M/I	3[b]	11	52	96	98	69	26	88	93	96
M/I[d]	3[b]	32	160	96	97	90	-	-	-	-
M/I	5[c]	10	89	78	78	1	64	264	20	78
A/B/T	3[a]	6	6	100	100	74	6	6	100	100
A/ B/T	4[b]	6	6	100	100	74	8	8	100	99
A/B/T	10[c]	20	20	100	100	0	64	68	9	99
A/B/T[e]	10[c]	20	-	-	-	-	20	20	100	-

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and binary interaction parameters (BIP's).
[d] For line search of axial BP's $M = 4$ for the component feed flow rate direction.
[e] For line search of axial BP's $M = 3$ for the BIP's direction.

3.5. Conclusions and recommendations

A modification of the OPT procedure, the SMSD procedure, for estimating PDR was developed and tested. Geometrical and distillation column design cases were used to compare the OPT and the SMSD procedures. The tests show that the ability of the SMSD procedure strongly depends on the CB's shape and number of parameters. For case studies with two uncertain parameters the SMSD procedure's computational efficiency is close to that of the OPT procedure. For some cases the SMSD procedure was able to compute more accurate PDR estimates with fewer models simulations, even when sometimes it required more BP's. For designs with more than two uncertain parameters the methodology is not able to approximate the constraint boundary accurately.

For designs with more than two uncertain parameters, the current SMSD procedure's approach for building the initial CBA underestimates considerably the actual CB. Modifications to the current approach may improve the performance of the procedure. These modifications may consider more initial BP's in addition to the axial BP's and an efficient method to connect them. Improvement of the line-search procedure to reduce the number of MS's per BP may help to make the method computationally efficient.

For designs with more than two uncertain parameters the OPT procedure is the most accurate and computationally efficient alternative. The initial tangential OPT PDR estimate's accuracy is usually within 8%. However this accuracy is compromised by the accuracy in BP's and tangent planes. The stand-alone distillation model simulator used in this work is not robust enough to provide invariably accurate BP's and tangent planes for the M/I design. The use of a commercial process simulator to perform the model simulations may be a better alternative.

For designs with more than two uncertain parameters the convergence criterion defined by Equation 2.28 cannot be used because of the considerable underestimation of the pessimistic CBA. Instead CMCI PDR estimates have been used to evaluate the convergence. However CMCI PDR estimates are usually unknown. Therefore, for designs with more than two uncertain parameters, the OPT procedure requires a more efficient way to evaluate the procedure's convergence.

References

MacDonald, R. J., 1993. An Accurate and Efficient Procedure for Estimating Design Reliability, Ph.D. Thesis, University of Kansas.

Chapter 4

Efficient Procedures for Estimating Process Design Reliability (PDR) Coupled with Commercial Process Simulator

Abstract

The certainty that a process will meet process constraints during normal operation despite the underlying uncertainty in process design parameters is the PDR. The identification of unnecessarily oversized or critically undersized equipment by PDR estimation and sensitivity analysis leads to better safety factor selection and appropriate capital investment. A computationally efficient tool to estimate PDR will be substantially more useful in a widely available design/rating tool, e.g. a commercial process simulator. This chapter describes two methods for coupling computationally efficient PDR estimating procedures with CHEMCAD 5.6.4. The chapter uses estimating PDR of distillation column designs as the example. This coupling makes reliability estimation available to practicing engineers.

4.1. Introduction

Process designers specify equipment to perform certain tasks, e.g. chemical reactions and separations. The designer must include experience-based safety factors when sizing the equipment because of inherent uncertainties and inaccuracies in the process model and design basis, (Capps and Thompson, 1983). However, the use of safety factors is not only often costly but also possibly ineffective or counterproductive. Optimal selection of safety factors requires rigorous calculation of the PDR. Monte Carlo integration (MCI) of the *c*-constraints mapped onto the *p*-parameter space is a computationally efficient methodology for estimating PDR (MacDonald, 1993; Howat, 1995). Ease of its

application and dissemination can be improved by coupling this method with CHEMCAD, a commercial process simulator widely used in the industry. This chapter describes the coupling of two versions of the Monte Carlo integration (MCI) of the *c*-constraints mapped onto the *p*-parameter space with CHEMCAD 5.6.4.

Chapter 2 discussed estimating PDR of multi-component distillation designs with conventional Monte Carlo integration (CMCI) and the optimistic-pessimistic-tangential (OPT) procedures. The OPT procedure required two to three orders of magnitude fewer model simulations (MS's) than the CMCI procedure did to compute accurate PDR estimates. However the OPT procedure's computational efficiency decreases as parameter dimension, with the commensurate boundary points (BP's), increases. This motivated the development and testing of a simplified version of the OPT procedure, the statistical most significant distance (SMSD) procedure.

Chapter 3 discussed the development and performance of the SMSD procedure. Initial testing of the SMSD procedure showed that it was computationally more efficient than the OPT procedure (Myers and Howat, 2005). This prompted the selection of the SMSD procedure to be coupled with CHEMCAD (Myers and Howat, 2005b). However, complete testing of the SMSD procedure showed that the procedure was unable to accurately estimate PDR for designs with more than two uncertain parameters. Because of this inability, the coupling of the SMSD procedure with CHEMCAD was not extended to analyze designs with more than two uncertain parameters. The development and testing of the SMSD procedure's coupling with CHEMCAD are described in this chapter.

The coupling of the OPT procedure with CHEMCAD was motivated by two circumstances. First, the SMSD procedure is limited to designs with two uncertain

parameters. Second, the stand-alone model simulator is limited and may cause inaccuracies in the OPT procedure results as discussed in Section 3.4. It was expected that the robustness of a commercial process simulator could help to provide more accurate BP's and tangents and hence improve the performance of the OPT procedure.

PDR estimation by CMCI procedure was a necessary precursor to evaluate the performance of the SMSD and OPT procedures coupled with CHEMCAD. The CMCI procedure was therefore integrated with CHEMCAD to provide the necessarily consistent comparison basis.

This chapter describes the coupling of the SMSD, CMCI and OPT procedures with CHEMCAD. The distillation column designs described in Chapter 2 are used as tests. The use of the PDR estimates for safety factor selection is demonstrated using a distillation column design for methanol purification.

4.2. CMCI

CMCI generates sets of random numbers, Monte Carlo (MC) sets, according to the parameter probability distributions and then performs a process simulation for each set to evaluate constraint compliance. The fraction of sets satisfying the constraints is a statistical estimator of the PDR. A probabilistic confidence interval for this estimator may be computed using Equation 2.9.

4.3. MCI of the *c*-constraints mapped onto the *p*-parameter space

The OPT and SMSD procedures evaluate PDR by MCI of the *c*-constraints mapped onto the *p*-parameter space. Both procedures map the constraint boundary (CB) in the

parameter space using a small set of boundary points (BP's) and geometrically interpolating among them. The OPT procedure uses two types of geometrical interpolations, tangential and connecting planes. The SMSD procedure uses only connecting planes. Both procedures are iterative. They start the constraint boundary approximation (CBA) using only the BP's located at the axial directions with respect to the nominal design. BP's are added to improve the PDR estimate and/or determine the convergence of the procedure. For designs with two uncertain parameters, both procedures are computationally more efficient than the CMCI procedure. Depending upon the CB shape, the SMSD procedure may be computationally more efficient than the OPT procedure is. For more than two uncertain parameters the SMSD procedure is not able to approximate the constraint boundary accurately, but the OPT procedure is. However as parameter dimension increases the OPT procedure's efficiency with respect to CMCI decreases. Chapter 2 and 3 describe in detail the OPT and SMSD procedures and their testing. Probabilistic confidence intervals for the OPT and SMSD PDR estimators may be computed using Equation 2.9.

4.4. CHEMCAD

CHEMCAD is a robust simulator that has the flexibility to allow users to couple it with their own computations by three different methods: user-added-module (AUM), EXCEL integration and parser unit operation. Conceptually, the three methods require the user to write code describing the module operation or analysis method. This code is subsequently linked with CHEMCAD making the module available to couple with other CHEMCAD calculations. The UAM method is the most powerful and fastest calculating

method out of the three options (CHEMCAD, 2007). A brief description of these methods follows.

4.4.1. User added module (AUM)

UAM's are developed using Microsoft's Visual C++ development tool, the same tools that were used in the creation of CHEMCAD unit operations. UAM's can be used to create new thermodynamic routines, unit operations or communicate data with other programs. UAM's are C++ functions compiled into a dynamic link library (DLL), USRADD.DLL. A Microsoft Visual C++ 5.0 project for compiling this DLL is provided by CHEMCAD to be customized by the users. This DLL project includes C++ functions to: 1) retrieve or set flow sheet data, 2) flash streams; and 3) calculate stream properties. The CHEMCAD 5.6.4 Microsoft Visual C++ 5.0 project allows users to create a maximum of ten unit operations: ADD1, ADD2, ADD3, …, and ADD10.

4.4.2. CHEMCAD EXCEL integration

CHEMCAD can be activated as an out-of-process server from Visual Basic Application (VBA) programs, e.g. EXCEL macros. This enables EXCEL to delegate computational tasks to CHEMCAD running in the background. CHEMCAD EXCEL integration can also be used for developing EXCEL unit operations. Customized user calculations or unit operations can be programmed as subroutines or functions using basic knowledge of Visual Basic (VB) and fundamental concepts like arrays and functions. CHEMCAD makes available CHEMCAD interface methods through a standard binary interface, i.e. component object module (COM). By executing interface methods the user

can 1) retrieve or set flowsheet data; 2) calculate simulations, K-values and enthalpy; 3) flash streams; and 4) convert engineering units. The calculations with this method are slower than the UAM method because of the interface between CHEMCAD and EXCEL. However, it is easier to implement than the UAM method.

4.4.3. Parser unit operation

Parser unit operations are defined using a C-like programming language (Parser). This method offers the power and flexibility of the high level C-like language without having to use a compiler. Parser unit operations are easily set up, but have limited flexibility compared to the other two methods.

4.4.4. Discussion

Successful results estimating PDR with the SMSD procedure for designs with two uncertain parameters motivated the coupling of this procedure with CHEMCAD (Myers and Howat, 2005b). The UAM method was selected for coupling because of its speed and flexibility.

CMCI PDR estimates were required for evaluating the performance of the SMSD procedure coupled with CHEMCAD. Coupling the CMCI procedure with CHEMCAD was necessary to provide the necessarily consistent comparison basis. The EXCEL integration method was selected for the coupling because it is easy to implement.

The OPT procedure was coupled with CHEMCAD to improve its performance and because it can be used for designs with more than two uncertain parameters. The EXCEL

integration method was selected for the coupling of the OPT procedure with CHEMCAD because it is easy to implement and modify.

The SMSD procedure coupled with CHEMCAD is limited to estimating the PDR of binary distillation columns with uncertainty in the components feed flow rates. However the CMCI and OPT procedures coupled with CHEMCAD also considers mixtures of three components and uncertainties in tray efficiency and binary interaction parameters (BIP's).

4.5. CMCI procedure coupled with CHEMCAD

VB code for the CMCI procedure was written in the EXCEL/VBA environment of an EXCEL file. The code was organized in VB subroutines and controlled by a main subroutine. The main functions of the code are: activate connection with CHEMCAD job, read input data from EXCEL file and CHEMCAD job, run a CHEMCAD model simulation for each MC set read from EXCEL file, compute CMCI statistics, and write results in EXCEL file. A CHEMCAD job is required for the model simulations and must contain a flowsheet with a SCDS distillation unit with one feed stream and two product streams. A description of the input/output data and instructions to set up a calculation and run the procedure are included and explained through an example.

4.5.1. Description of the CMCI procedure's VB code

A main VB subroutine was programmed to execute the CMCI procedure's sequential and iterative computations. This main subroutine calls sequentially five subroutines to read input data and then execute the loop with the CMCI procedure's iterative

computations. Table 4.1 describes the computations of each of the five subroutines and the loop. The computations of the subroutines listed in Table 4.1 are actually broken into simpler subroutines. The complete list and description of subroutines of the CMCI procedure coupled with CHEMCAD may be found in Appendix A.

Chapter 2 discussed the importance of using good quality random numbers in Monte Carlo integration and tested the quality of the random numbers generated by the FORTRAN IMSL libraries. Because of that, it was desired to use the same libraries for the work presented in this Chapter. For this, three FORTRAN subroutines that use the FORTRAN IMSL libraries were compiled into a FORTRAN DLL, DLLFORCMCI.dll, such that they could be accessed by VB code. One of the subroutines generates random numbers from independent normal distributions. Another of the subroutines generates random numbers from a uniform distribution. The last subroutine generates random sets from correlated normal distributions. Then three EXCEL VB subroutines were written to call the FORTRAN subroutines. Input data for these subroutines are read from the EXCEL file. Output data, i.e. random sets, are written into one of the worksheets of the EXCEL file.

Table 4.1. Description of computations of subroutines in the CMCI procedure's code.

Subroutine name or loop	Description of computations
LoadCC5	• Reads from EXCEL file path to find CHEMCAD job and activates connection with CHEMCAD job. • Reads flowsheet topography from EXCEL file. • Gets from CHEMCAD job number of components, component names and component molecular weights. Writes information in EXCEL file. • Reads from EXCEL file the types of parameter uncertainty, computes the total number of uncertain parameters and displays it in EXCEL file.
IniStreamDat	• Reads from EXCEL file nominal component feed flow rates and sets values in CHEMCAD job. • Reads nominal tray efficiency and BIP's from EXCEL file or CHEMCAD job, depending upon what the user selects to do. If values are read from the EXCEL file then the values are set in CHEMCAD job, otherwise the inverse procedure is done. . • Reads feed stream pressure from EXEL file and sets value in CHEMCAD job. • Uses CHEMCAD interface to flash feed stream in CHEMCAD job. • Reads statistical description of the uncertain parameters from EXCEL file.
SetNominalUnitopSpec	• Reads from EXCEL file nominal design condenser and reboiler specifications and sets values in CHEMCAD job. • Runs CHEMCAD nominal design simulation. Retrieves from CHEMCAD job computed reboiler duty and writes results in EXCEL file.
SetControlVariables	• Reads from EXCEL file control variables to use for PDR estimation and sets values in CHEMCAD job.
ConstReadInfo	• Reads from EXCEL file process constraint specifications.
Loop	• Reads MC set in turn, from EXCEL file and sets values in CHEMCAD job. • Runs the CHEMCAD model simulation and gets results from CHEMCAD job to evaluate process constraints to determine if MC set is inside or outside the success region. • Compute CMCI PDR estimate and 95% confidence interval.

The CMCI procedure's code coupled with CHEMCAD has the following limitations:

1. The code only considers a maximum of three components and three pairs of BIP's.

However, the code can be modified to extend the application for more components.

2. The code considers only one feed stream to the distillation column and two products, top and bottom.
3. Only the following five process constraint specification options are considered: 1) minimum top product purity, 2) maximum bottom product impurity, 3) maximum component mass flow rate in bottom product, 4) maximum mass fraction (dry basis) of component one in top product, and 5) maximum ppmw of one component in top product.
4. The maximum number of MC sets is limited by the EXCEL worksheet's maximum number of rows which varies with the EXCEL version. However the code may be modified to increase the number of MC sets by using additional EXCEL columns.

4.5.2. Input data set up and calculation example

The example considers a distillation column to separate an acetone/benzene (A/B) mixture. Table 4.2 contains the nominal design specifications for the column.

Table 4.2. Nominal design specifications for example A/B distillation column.

Stages	25
Feed stage	15
Feed state	Sat. liquid
Component feed flow rates	500 lbmol/hr A, 500 lbmol/hr B
Condenser pressure	15 psia
Vapor overhead	18 psia
Pressure drop / stage	0.1 psi
Top product recovery	80% A
Top product	$x_A \geq 95$
Tray efficiency	60%
BIP's (TK-Wilson model)	$\lambda_{12} - \lambda_{11} / \lambda_{21} - \lambda_{22} = 577.47 / -234.41$

The CHEMCAD job with flow sheet is created first because the EXCEL file requires it. Figure 4.1 shows the CHEMCAD job's flowsheet for the example. The distillation

module is set up in the conventional steady state manner.

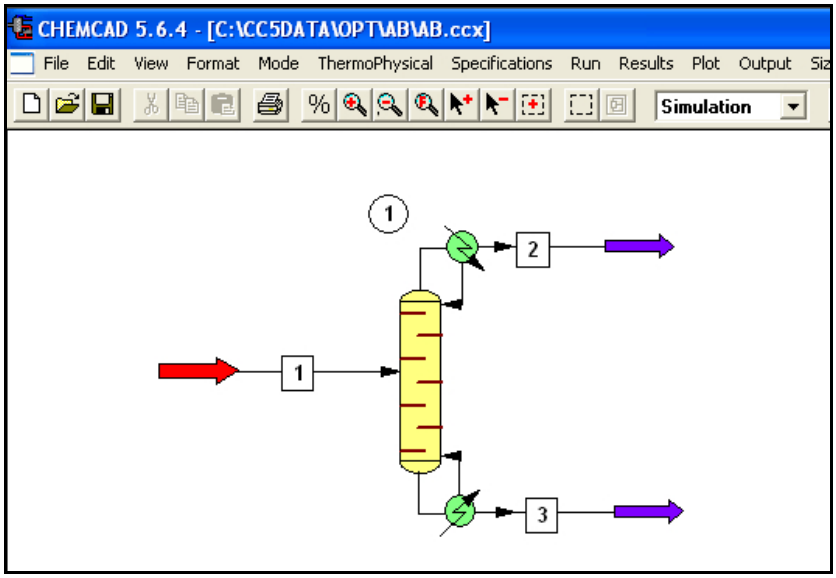


Figure 4.1. CHEMCAD flowsheet for PDR estimation by CMCI procedure.

The example assumes uncertainty in component feed flow rates, tray efficiency and BIP's. The statistical description of the parameter uncertainty is given in Table 4.3.

Table 4.3. Statistical description of parameter uncertainty.

Component feed flow rates (uncorrelated normal distributions)	Component	A	B
	Mean (lbmol/hr)	500	500
	Standard deviation (lbmol/hr)	100	100
Tray efficiency (uniform distribution)	Minimum (%)	50	
	Maximum (%)	60	
BIP's (correlated normal distributions)	Pair	$\lambda_{12}-\lambda_{11}$	$\lambda_{21}-\lambda_{22}$
	Mean (cal/gmol)	577.47	–234.41
	Standard deviation (cal/gmol)	49.706	31.409
	Correlation coefficient	–0.992799	

For PDR estimation, a 25% safety factor in reboiler duty is used. Reboiler duty and top product recovery are used as control variables. These control variables, which give operating flexibility to meet process constraints, are set to their limiting values to reduce the burden of the problem. The process constraints are 95 mol% minimum A in top product and 25 mol% maximum A in bottom product.

The starting EXCEL file must contain the CMCI procedure's code and the file's worksheets must be formatted to be compatible with the code. Starting with an EXCEL file previously used by another design calculation ensures this. The EXCEL file is located in the same directory as the CHEMCAD job subdirectory for ease of localization. Figure 4.2 shows a screen shot of a worksheet of the starting file used for the example. The file had been used for estimating the PDR of a distillation column to separate an acetone/water mixture. Cells with gray background contain input data that must be entered by the user.

Preparing the worksheet for running the CMCI procedure involves six sequential steps. The first five steps involve entering data for each of the subroutines described in Table 4.1 and running the first four subroutines after entering the data. The last step involves generating or verifying the availability of the required MC sets and running the CMCI procedure. The summary of data that must be entered by the user is listed in Table 4.4. The six steps are described below.

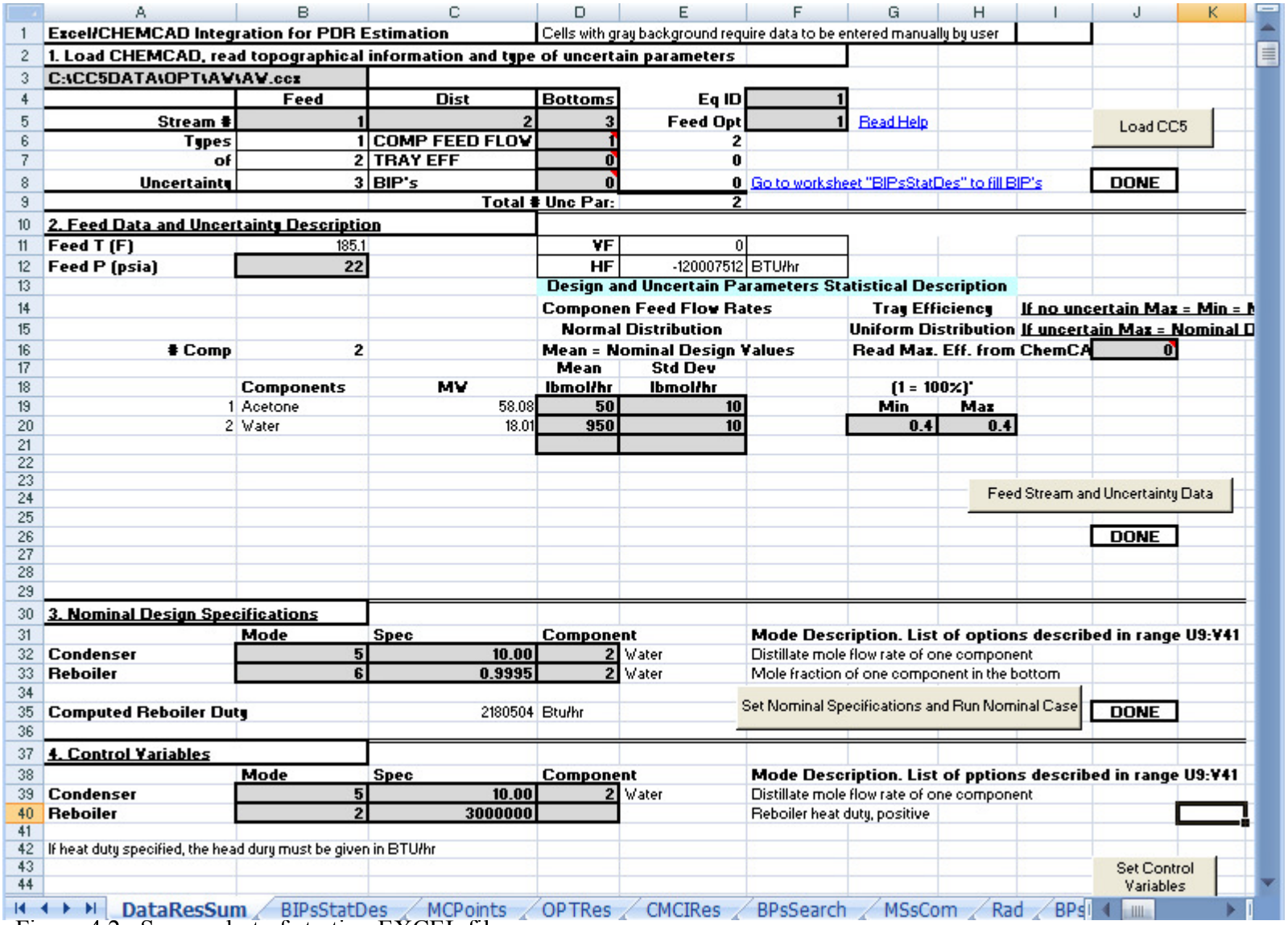


Figure 4.2. Screen shot of starting EXCEL file.

Table 4.4. Input data in EXCEL spreadsheet.

Seccion 1.		
Path	C:\CC5DATA\OPT\AB\AB.ccx	
Feed stream number	1	
Distillate stream number	2	
Bottoms stream number	3	
Equipment ID	1	
Feed option	1	
Types of uncertainty	Comp. feed flow rates, tray efficiency and BIP's	
Seccion 2.		
Feed pressure	20 psia	
Nominal uncertain parameter values	Data in Table 4.2	
Read max eff. from CHEMCAD	0	
Read BIP's from CHEMCAD	0	
Uncertainty statistical description	Data in Table 4.3	
Seccion 3.		
Nominal condenser specification	Comp. mole fraction in distillate, 0.95 of A	
Nominal reboiler specification	Comp. recovery in bottom product, 0.20 of A	
Seccion 4.		
Condenser control variable	Comp. recovery in distillate, 0.80 of A	
Reboiler control variable	Reboiler duty, 23670020 Btu/hr	
Seccion 5.		
Distillate constraint specification	Comp. mole fraction, $\geq$ 0.95 of A	
Bottoms constraint specification	Comp. mole fraction, $\leq$ 0.25 of A	
Seccion 6.		
Run again steps 1-4	1	
Maximum step in linear search	3 σ	
MC sets	10000	
Maximum iterations	15	
Extra-results ouput	0	0

1. Entering data for subroutine "LoadCC5" and running it. Figure 4.3 shows a screen shot of the section of the EXCEL file worksheet "DataResSum" for input data for the subroutine. The cells with gray background have been updated with the example's data. After entering data, the button labeled "Load CC5" is clicked to run the subroutine.

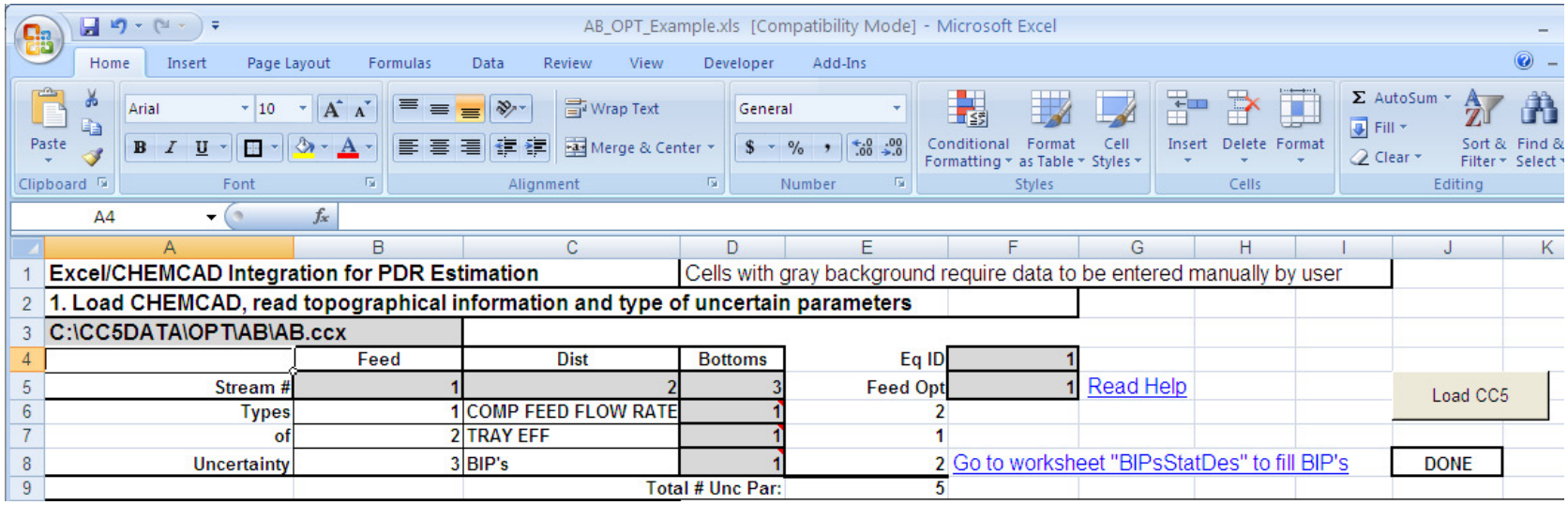
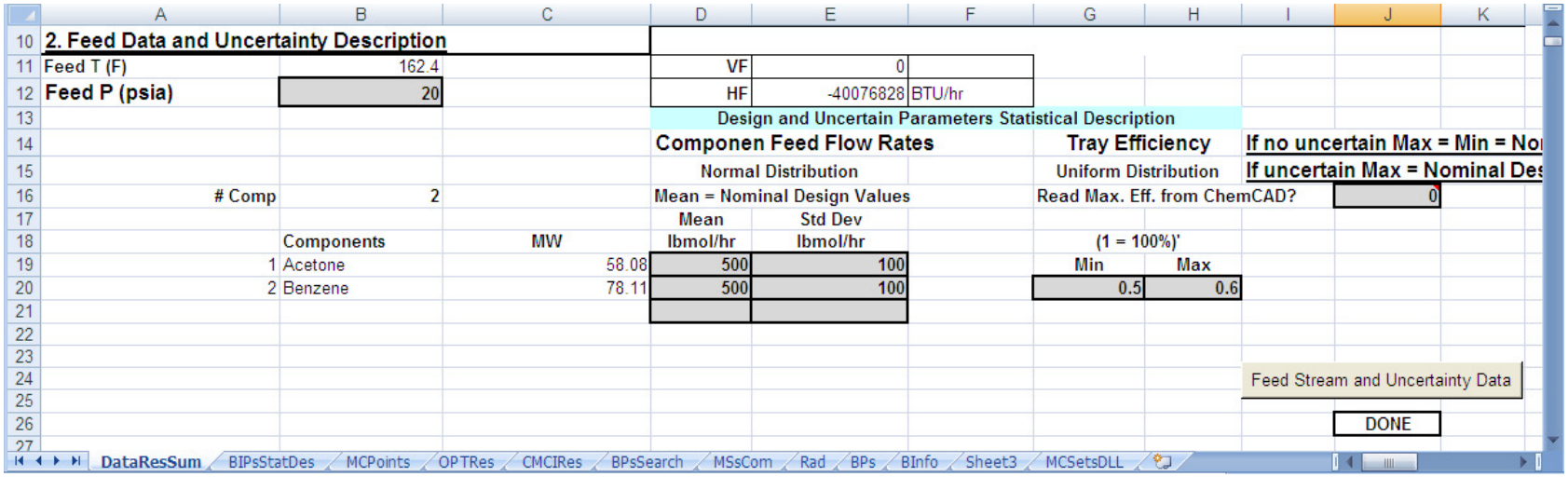


Figure 4.3. Screen shot showing input data for subroutine LoadCC5.

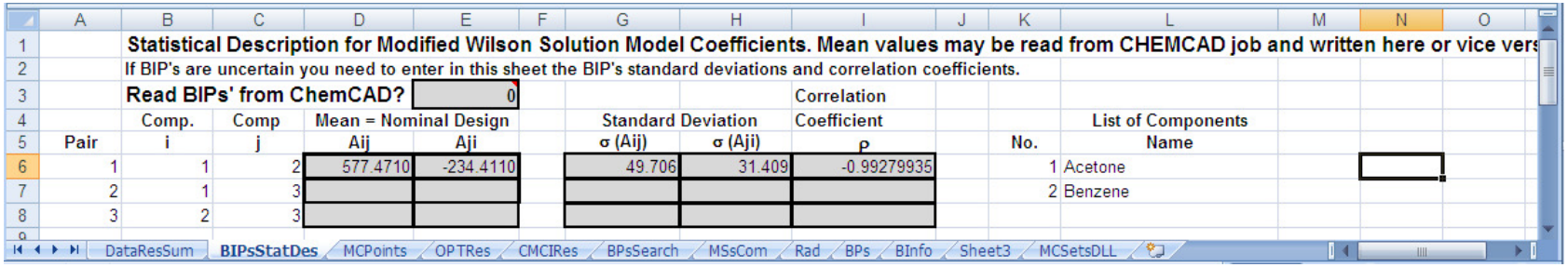
2. Entering data for subroutine “IniStreamDat” and running it. Figures 4.4 and 4.5 show screen shots of the sections of the EXCEL file worksheets “DataResSum” and “BIPsStatDes” that contain input data for the subroutine. The cells with gray background have been updated with the example’s input data. After updating data, the button labeled “Feed Stream and Uncertainty Data” is clicked to run the subroutine.
3. Entering data for subroutine “SetNominalUnitopSpec” and running it. Figure 4.6 shows a screen shot of the worksheet “DataResSum” that contains the input data for the subroutine, i.e. condenser and reboiler specifications. This calculation is not essential for the PDR calculations. However the designer may use the results to establish values for safety factors. The options for condenser and reboiler specifications are those available by CHEMCAD for the SCDS unit and listed in Table 4.5. The cells with gray background have been updated with the example’s input data. For this example the condenser and reboiler specifications are component specifications in the top and bottom products. Component numbers are either found in the CHEMCAD job or in the input data section of step 2. For instance, for component A is displayed in cell A19 of worksheet “DataResSum”, see Figure 4.4. If the condenser or reboiler specification is heat duty, the cell with component number would be left empty. After entering the nominal design specifications, the subroutine is run by clicking the button labeled “Set Nominal Specifications and Run Nominal Case”.



10	2. Feed Data and Uncertainty Description												
11	Feed T (F)	162.4		VF	0								
12	Feed P (psia)	20		HF	-40076828	BTU/hr							
13				Design and Uncertain Parameters Statistical Description									
14				Componen Feed Flow Rates			Tray Efficiency		If no uncertain Max = Min = No				
15				Normal Distribution			Uniform Distribution		If uncertain Max = Nominal Des				
16	# Comp	2		Mean = Nominal Design Values			Read Max. Eff. from ChemCAD?		0				
17				Mean	Std Dev								
18		Components	MW	lbmol/hr	lbmol/hr		(1 = 100%)'						
19	1	Acetone	58.08	500	100		Min	Max					
20	2	Benzene	78.11	500	100		0.5	0.6					
21													
22													
23													
24									Feed Stream and Uncertainty Data				
25													
26									DONE				
27													

DataResSum | BIPsStatDes | MCPoints | OPTRes | CMCIRes | BPsSearch | MSsCom | Rad | BPs | BInfo | Sheet3 | MCSetsDLL

Figure 4.4. Screen shot of worksheet "DataResSum" showing input data for subroutine "IniStreamDat".



1	Statistical Description for Modified Wilson Solution Model Coefficients. Mean values may be read from CHEMCAD job and written here or vice vers												
2	If BIP's are uncertain you need to enter in this sheet the BIP's standard deviations and correlation coefficients.												
3	Read BIPs' from ChemCAD?	0						Correlation					
4		Comp.	Comp	Mean = Nominal Design			Standard Deviation		Coefficient			List of Components	
5	Pair	i	j	Aij	Aji		σ (Aij)	σ (Aji)	ρ		No.	Name	
6	1	1	2	577.4710	-234.4110		49.706	31.409	-0.99279935		1	Acetone	
7	2	1	3								2	Benzene	
8	3	2	3										

DataResSum | BIPsStatDes | MCPoints | OPTRes | CMCIRes | BPsSearch | MSsCom | Rad | BPs | BInfo | Sheet3 | MCSetsDLL

Figure 4.5. Screen shot of worksheet "BIPsStatDes" showing input data for subroutine "IniStreamDat".

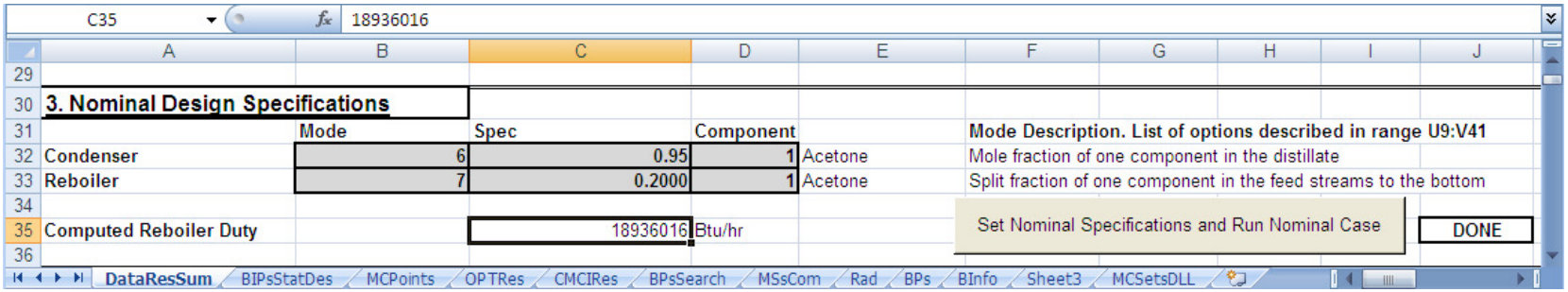


Figure 4.6. Screen shot from worksheet “DataResSum” showing input data for subroutine “SetNominalUnitopSpec”.

Table 4.5. Condenser and reboiler specification options for CHEMCAD SCSD model.

Condenser		Reboiler	
0	No condenser	0	No reboiler
1	Reflux ratio	1	Boil-up ratio V/B
2	Condenser heat duty, negative	2	Reboiler heat duty, positive
3	Condenser temperature	3	Reboiler temperature
4	Total distillate mole flow rate	4	Total bottom mole flow rate
5	Distillate mole flow rate of one component	5	Bottom mole flow rate of one component
6	Mole fraction of one component in the distillate	6	Mole fraction of one component in the bottom
7	Split fraction of one component in the feed streams to the distillate	7	Split fraction of one component in the feed streams to the bottom
8	Fractional amount of feeds in the distillate	8	Fractional amount of feeds in bottom
9	Molar flow ratio between two components in the distillate	9	Molar flow ratio between two components in the bottom
10	Distillate mass flow rate	10	Bottom mass flow rate
11	Distillate component mass flow rate	11	Bottom component mass flow rate
12	Distillate component mass fraction	12	Bottom component mass fraction
13	Distillate std liquid volume flow rate		
14	Reflux mole flow rate		
15	Reflux mass flow rate		

4. Entering data for subroutine “SetControlVariables” and running subroutine. Figure 4.7 shows a screen shot of the worksheet “DataResSum” that contains the input data for the subroutine, i.e. condenser and reboiler specifications. The options for condenser and reboiler specifications are those listed in Table 4.5. The cells with gray background have been updated. After updating the data, the subroutine is run by clicking the button labeled “Set Control Variables”.
5. Entering process constraint specifications for subroutine “ConstReadInfo”. Figure 4.8 shows a screen shot of the worksheet “DataResSum” that contains the input data for the subroutine. The example’s constraint specifications have been updated. There is no button to run the subroutine. The subroutine is called by the CMCI procedure’s code.

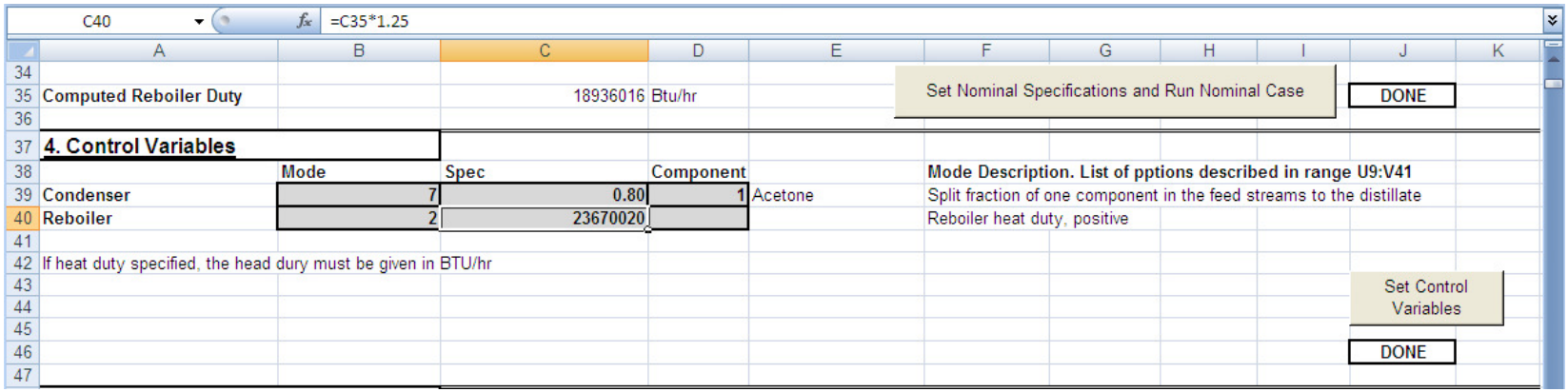


Figure 4.7. Screen shot from worksheet "DataResSum" showing input data for subroutine "SetControlVariables".

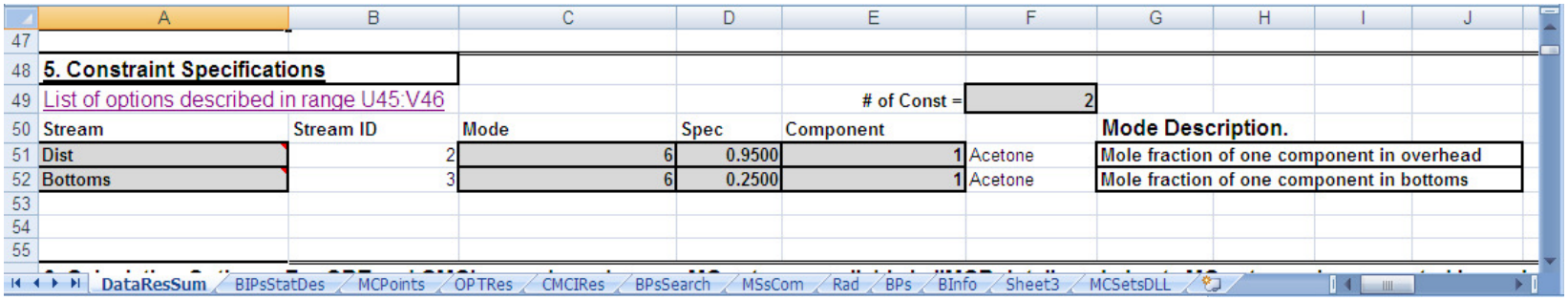


Figure 4.8. Screen shot from worksheet "DataResSum" showing input data for subroutine "ConstReadInfo".

6. Choosing calculation options, checking MC sets availability, and running procedure. The middle section of Figure 4.9 shows the input options for running the CMCI procedure. The user can chose to run again the first four subroutines described in Table 4.1. It is recommended to select to run the first four subroutines again to ensure any changes have been updated. The user can also choose if the constraints' values for each MC set are written in the results area of the worksheet "CMCIRes". Those values are necessary if the designer wants to analyze the results in detail but typically those values are not necessary. If the user does not need those values is recommended to not write them to reduce computing time. The user must enter the number of MC sets to use. The first time that the CMCI procedure is run for a case study, the MC sets need to be generated and copied to the worksheet "MCPoints". Figure 4.10 shows the first ten MC sets in the worksheet "MCPoints" for this example. Below it is described how the MC sets are obtained. After updating the data, the button labeled "CMCI" is clicked to run the CMCI procedure. The code writes the CMCI procedure's results in the worksheet "DatResSum" and "CMCIRes". The results written in the worksheet "DatResSum" is a summary of the computations. It includes the PDR evaluated with the total of MC sets, the number of uncertain parameters, the date, initial and final time of the computations, and computing time. For this example, the CMCI procedure estimated 82% PDR. The calculation used 10,000 MC sets and took 553 s.

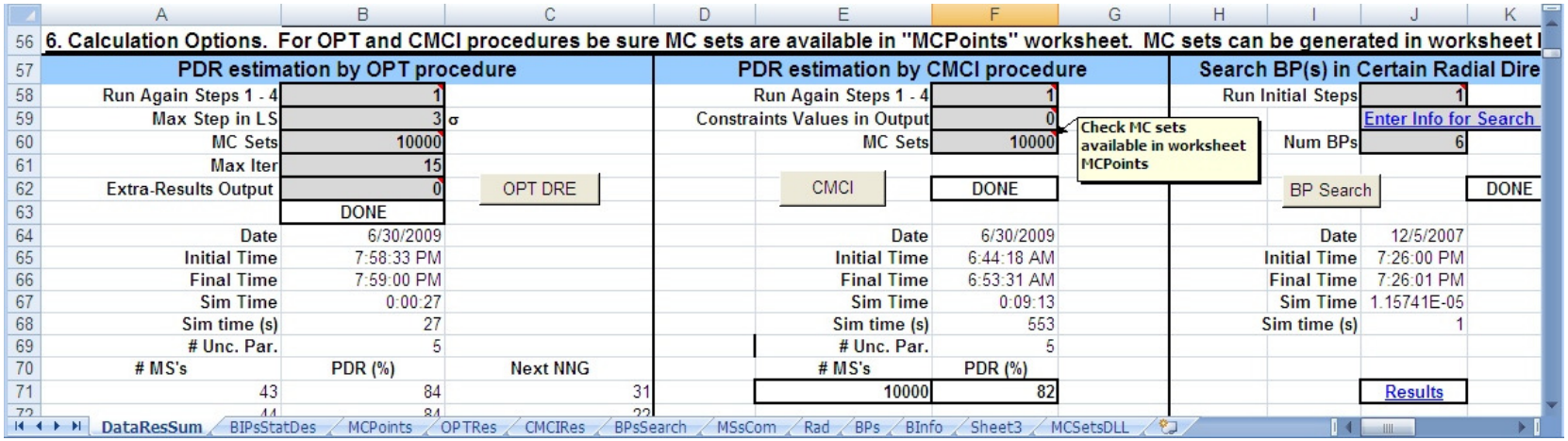


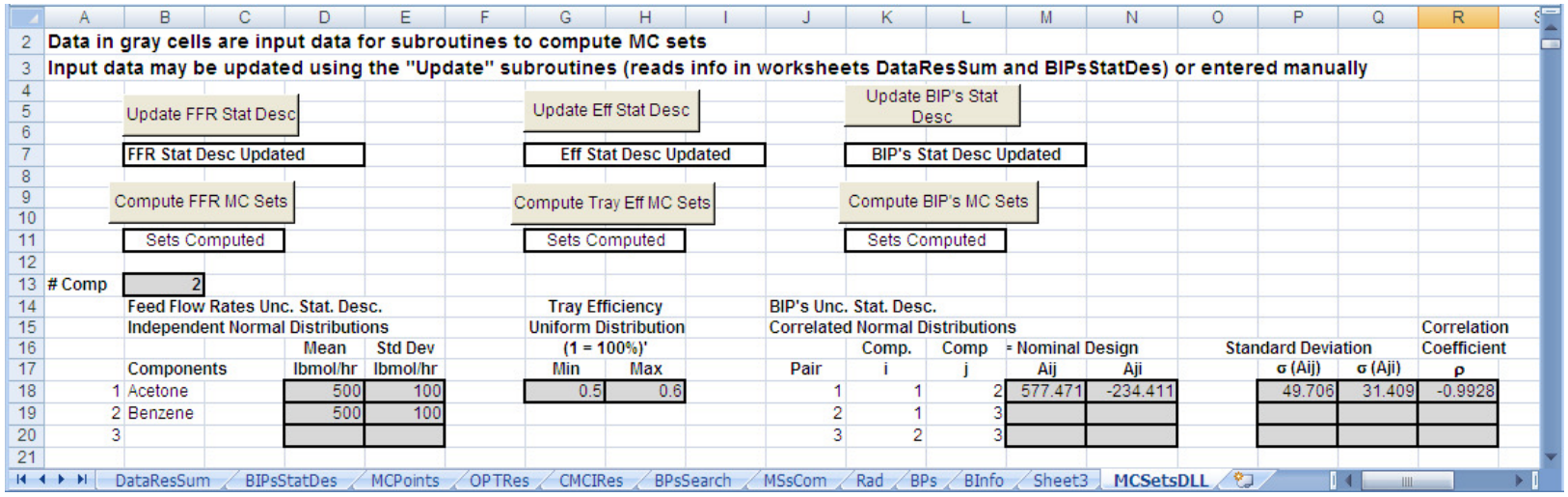
Figure 4.9. Screen shot from worksheet "DataResSum" showing calculation options. The CMCI procedure's options are shown in the middle section.

	A	B	C	D	E	F	G	H
1	OPT (In/out)	ffr1	ffr2	eff	BIP12	BIP21	7:59:03 PM	6/30/2009
2	0	705.157	474.866	0.536	651.772	-279.288		
3	1	608.325	482.305	0.549	518.969	-198.482		
4	0	508.256	634.298	0.525	602.565	-250.099		
5	1	627.773	407.081	0.578	593.036	-242.628		
6	1	377.404	561.566	0.554	569.126	-230.821		
7	1	533.853	384.172	0.591	585.149	-237.332		
8	1	367.990	368.480	0.598	590.835	-240.719		
9	1	347.555	420.681	0.544	610.347	-255.205		
10	1	454.076	332.728	0.532	585.975	-241.273		

DataResSum BIPsStatDes MCPoints OPTRes CMCIRes BPsSearch MSsCon

Figure 4.10. Screen shot from worksheet "MCPoints" showing the first ten MC sets.

Figure 4.11 shows a screen shot of the worksheet "MCSetsDLL" which is used for the input and output when generating MC sets. The screen shot shows the worksheet's section with the input data for generating MC sets for component feed flow rates, tray efficiency, and BIP's. The input data are the statistical descriptions of the uncertain parameters and are contained in the cells with gray background. When the component feed flow rates' uncertainty statistical descriptions are the same as those entered in the worksheet "DatResSum", the button labeled "Update FFR Stat Desc" may be clicked to copy the information from worksheet "DatResSum" to worksheet "MCSetsDLL". The same may be done for the tray efficiency and BIP's using the buttons labeled "Update Eff Stat Desc", and "Update BIP's Stat Desc", respectively. In the case of the BIP's the data is read from the worksheet "BIPsStatDes". After the input data have been updated, the MC sets for component feed flow rates, tray efficiency and/or BIP's may be generated by clicking the buttons "Compute FFR MC Sets", "Compute Tray Eff MC Sets", and/or "Compute BIP's MC Sets", respectively. Figure 4.12 shows a screen shot of a section of the worksheet "MCSetsDLL" containing few of the generated MC sets.



Data in gray cells are input data for subroutines to compute MC sets

Input data may be updated using the "Update" subroutines (reads info in worksheets DataResSum and BIPsStatDes) or entered manually

Update FFR Stat Desc | FFR Stat Desc Updated | Update Eff Stat Desc | Eff Stat Desc Updated | Update BIP's Stat Desc | BIP's Stat Desc Updated

Compute FFR MC Sets | Sets Computed | Compute Tray Eff MC Sets | Sets Computed | Compute BIP's MC Sets | Sets Computed

Comp: 2

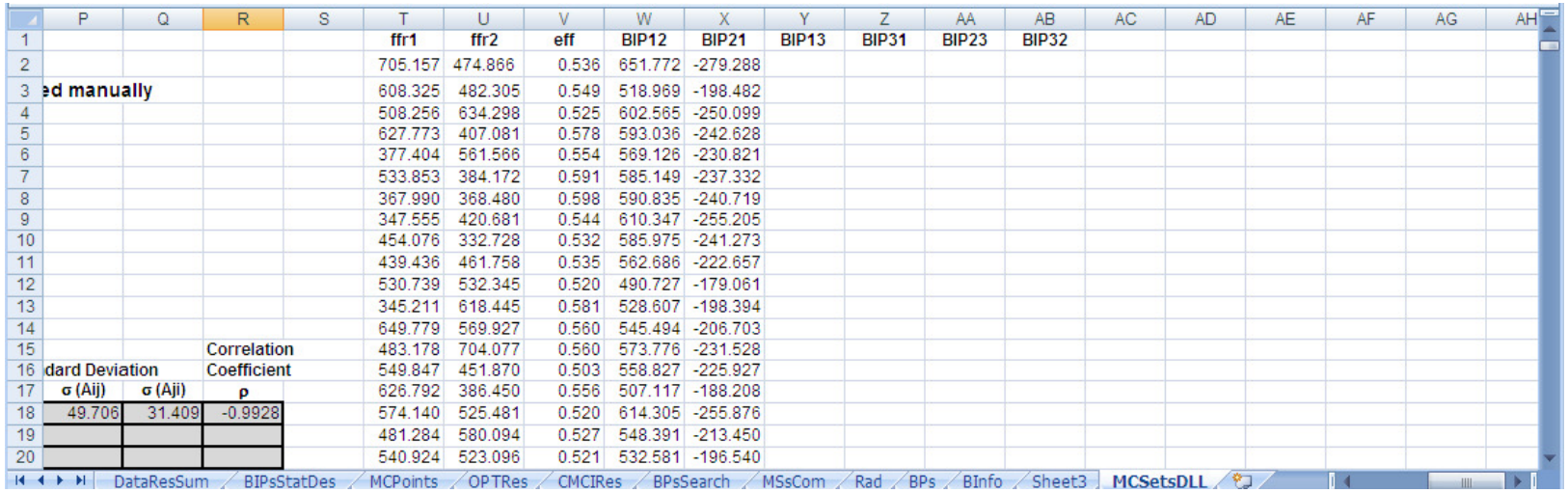
	Components	Feed Flow Rates Unc. Stat. Desc. Independent Normal Distributions Mean lbmol/hr	Std Dev lbmol/hr
1	Acetone	500	100
2	Benzene	500	100
3			

Tray Efficiency Uniform Distribution (1 = 100%)' Min	Max
0.5	0.6

BIP's Unc. Stat. Desc. Correlated Normal Distributions Pair	Comp. i	Comp j	= Nominal Design Aij	Aji	Standard Deviation σ (Aij)	σ (Aji)	Correlation Coefficient ρ
1	1	2	577.471	-234.411	49.706	31.409	-0.9928
2	1	3					
3	2	3					

DataResSum | BIPsStatDes | MCPoints | OPTRes | CMCIRes | BPsSearch | MSsCom | Rad | BPs | BInfo | Sheet3 | MCSetsDLL

Figure 4.11. Screen shot from worksheet "MCSetsDLL" showing the input data section to generate MC sets.



ffr1	ffr2	eff	BIP12	BIP21	BIP13	BIP31	BIP23	BIP32
705.157	474.866	0.536	651.772	-279.288				
608.325	482.305	0.549	518.969	-198.482				
508.256	634.298	0.525	602.565	-250.099				
627.773	407.081	0.578	593.036	-242.628				
377.404	561.566	0.554	569.126	-230.821				
533.853	384.172	0.591	585.149	-237.332				
367.990	368.480	0.598	590.835	-240.719				
347.555	420.681	0.544	610.347	-255.205				
454.076	332.728	0.532	585.975	-241.273				
439.436	461.758	0.535	562.686	-222.657				
530.739	532.345	0.520	490.727	-179.061				
345.211	618.445	0.581	528.607	-198.394				
649.779	569.927	0.560	545.494	-206.703				
483.178	704.077	0.560	573.776	-231.528				
549.847	451.870	0.503	558.827	-225.927				
626.792	386.450	0.556	507.117	-188.208				
574.140	525.481	0.520	614.305	-255.876				
481.284	580.094	0.527	548.391	-213.450				
540.924	523.096	0.521	532.581	-196.540				

ed manually

dard Deviation: σ (Aij) 49.706 | σ (Aji) 31.409 | Correlation Coefficient ρ -0.9928

DataResSum | BIPsStatDes | MCPoints | OPTRes | CMCIRes | BPsSearch | MSsCom | Rad | BPs | BInfo | Sheet3 | MCSetsDLL

Figure 4.12. Screen shot from worksheet "MCSetsDLL" showing generated MC sets.

4.5.3. Case studies and results

The case studies for the evaluation of the procedures presented in this chapter are similar to the cases described in Chapter 2 with data presented in Table 2.1. For testing the procedures coupled with CHEMCAD a modification was required for the A/B, M/I and acetone/benzene/toluene (A/B/T) designs. Table 2.1 lists reboiler vapor rate as one of the control variable column specifications for those three designs. However the CHEMCAD SCDS distillation column unit does not allow reboiler vapor rate as a design specification. Therefore, reboiler heat duty was used instead for the three designs. Table 4.6 lists the reboiler heat duty specifications for the three designs used for the PDR estimations.

Table 4.6. Modification to distillation case studies for the tests with CHEMCAD coupling.

Specifications \ Mixture	A/B	M/I	A/B/T
Reboiler heat duty	2.4E06 Btu/hr	1.4E06 Btu/hr	1.9E6 Btu/hr

Tables 4.7 and 4.8 list the PDR estimates and 95% CI lengths computed by the CMCI procedure coupled with CHEMCAD using different MC set sizes, respectively. The PDR estimates are consistent with the results presented in Table 2.3 obtained with the stand-alone CMCI procedure. For cases with PDR's greater than 95%, MC set sizes of 1,000 or less are enough to converge to accurate PDR estimates. However, more than 1,000 sets may be required to reduce their CI's to an acceptable value. For cases with PDR's lower than 95%, an excess of 1,000 random sets or more are required to obtain accurate PDR estimates. Table 4.9 lists PDR estimates, 95% confidence intervals (CI's) and computing time for two sizes of MC sets. The results demonstrate the excessive computational cost to obtain accurate PDR estimates.

Table 4.7. CMCI PDR evaluated with different random number set sizes.

Mixture	# Par	PDR Estimate (%)					
		100 sets	500 sets	1000 sets	2000 sets	5000 sets	10000 sets
A/B	2[a]	84	89	90	91	91	91
A/B	3[b]	72	77	80	81	81	81
A/B	5[c]	73	77	80	82	82	82
A/W	2[a]	87	91	93	93	94	93
A/W	3[b]	53	62	67	67	68	68
A/W	5[c]	53	62	67	67	68	68
M/I	2[a]	98	98	98	98	99	98
M/I	3[b]	94	95	96	96	97	97
M/I	5[c]	82	81	81	81	81	81
A/B/T	3[a]	100	99	99	100	100	100
A/ B/T	4[b]	100	99	99	100	100	100
A/B/T	10[c]	100	99	100	100	100	100

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and binary interaction parameters.

Table 4.8. CMCI PDR 95% CI length evaluated for different random number set sizes.

Mixture	# Par	95% CI					
		100 sets	500 sets	1000 sets	2000 sets	5000 sets	10000 sets
A/B	2[a]	14.3	5.5	3.8	2.5	1.6	1.1
A/B	3[b]	17.3	7.4	5.0	3.4	2.2	1.5
A/B	5[c]	17.2	7.3	4.9	3.4	2.1	1.5
A/W	2[a]	13.2	5.0	3.2	2.2	1.4	1.0
A/W	3[b]	19.2	8.5	5.8	4.1	2.6	1.8
A/W	5[c]	19.2	8.5	5.8	4.1	2.6	1.8
M/I	2[a]	6.5	2.6	1.7	1.1	0.7	0.5
M/I	3[b]	9.7	3.7	2.4	1.7	1.0	0.7
M/I	5[c]	15.0	6.8	4.8	3.4	2.2	1.5
A/B/T	3[a]	3.7	1.7	1.0	0.6	0.4	0.3
A/ B/T	4[b]	3.7	1.7	1.0	0.6	0.4	0.3
A/B/T	10[c]	3.7	1.5	1.0	0.6	0.3	0.2

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and binary interaction parameters.

Table 4.9. PDR estimates from CMCI procedure coupled with CHEMCAD for two sizes of MC sets.

Mixture	*P*	1,000 MC sets			10,000 MC sets		
		PDR (%)	95% CI	Time (s)	PDR (%)	95% CI	Time (s)
A/B	2[a]	90	88 - 91	55	91	90 - 91	524
A/B	3[b]	80	77 - 82	52	81	81 - 82	502
A/B	5[c]	80	78 - 83	52	82	81 - 82	520
A/W	2[a]	93	91 - 94	46	93	93 - 94	406
A/W	3[b]	67	64 - 69	48	68	67 - 69	452
A/W	5[c]	67	64 - 70	52	68	67 - 69	475
M/I	2[a]	98	97 - 99	267	98	98 - 99	2808
M/I	3[b]	96	95 - 97	274	97	96 - 97	2810
M/I	5[c]	81	79 - 84	220	81	81 - 82	2311
A/B/T	3[a]	99	99 - 100	52	100	99 - 100	523
A/ B/T	4[b]	99	99 - 100	57	100	99 - 100	510
A/B/T	10[c]	100	99 - 100	60	100	99 - 100	589

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and BIP's.

4.6. SMSD procedure coupled with CHEMCAD

The SMSD procedure's code needed to be restructured such that a CHEMCAD flowsheet could be set up. The flow sheet should allow for the sequential and iterative computations of the SMSD procedure. Also the flow sheet should include a distillation unit for the model simulations. Figure 4.13 presents a flow chart with the main calculations of the SMSD procedure. This is a restructured version of the flow chart presented in Chapter 3. This flow chart indicates two nested loops of iterative computations. An outer loop for adding BP's to the CBA and an internal loop for the search of BP's, i.e. line-search procedure. The CHEMCAD distillation unit is located inside the internal loop.

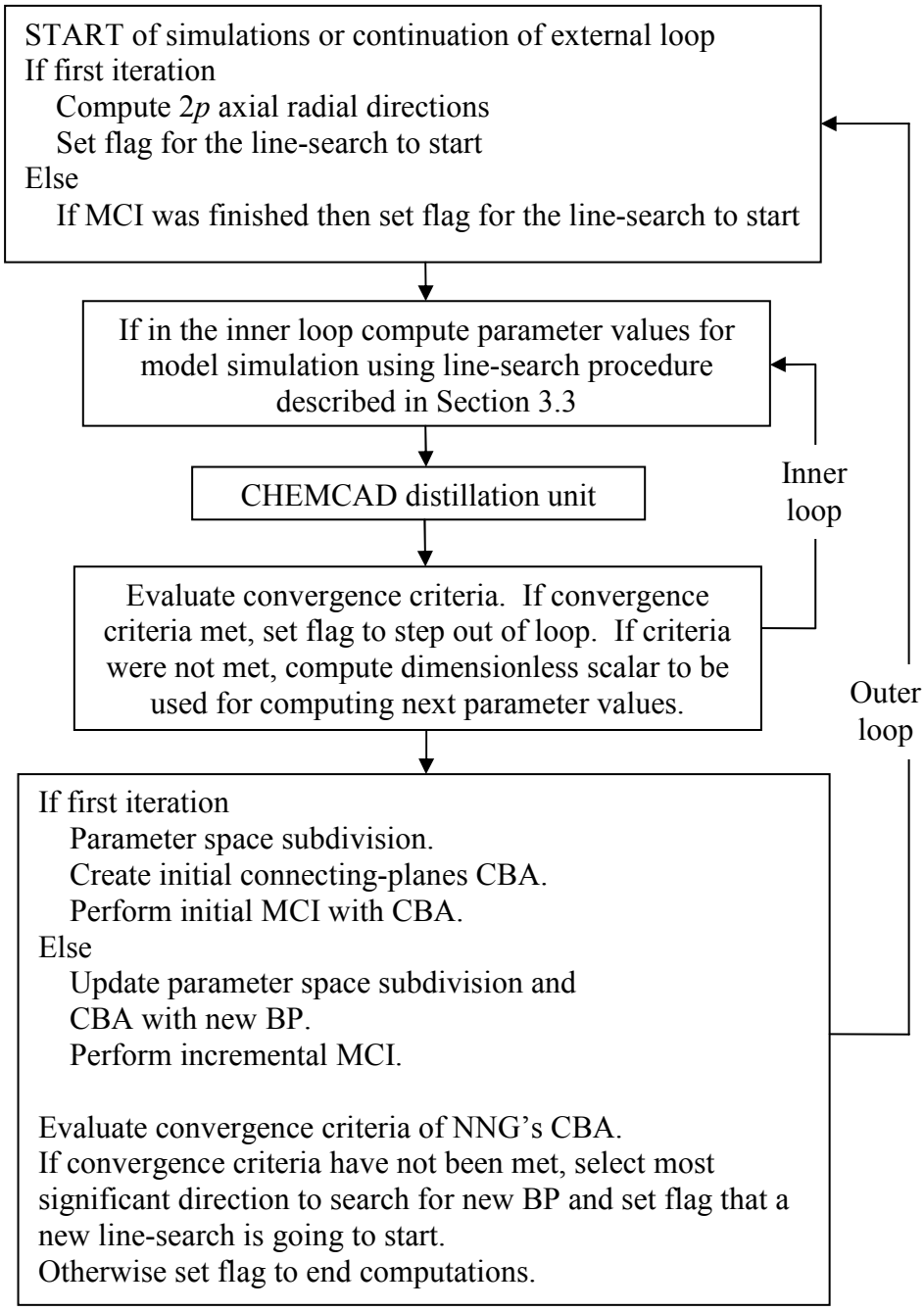


Figure 4.13. Flow chart of SMSD procedure to estimate PDR

The SMSD procedure's code was divided into four UAM's to meet the requirements described above. Figure 4.14 shows a CHEMCAD flow sheet with the four developed UAM's to estimate the PDR of a binary distillation column by the SMSD procedure. Modules ADD8 and ADD9 are used for the inner loop computations and modules ADD6 and ADD7 are used for the external loop computations. The recycle streams in the flow sheet are used to control the iterative calculations. Modifying the recycle stream's data signals CHEMCAD to stay in the loop formed by the recycle stream. Keeping the recycle stream's data constant signals CHEMCAD to exit the loop and continue with the following sequence of computations. Stream 1 is used to hold the distillation column's component feed flow rates at nominal conditions. Streams 2, 3, and 4 are used by the line-search procedure. Stream 2 is used to hold the trial component feed flow rates. Stream 3 and/or 4 may be used to evaluate the convergence criteria of the line-search procedure. Data in streams 6, 7, and 8 are not relevant for the SMSD computations.

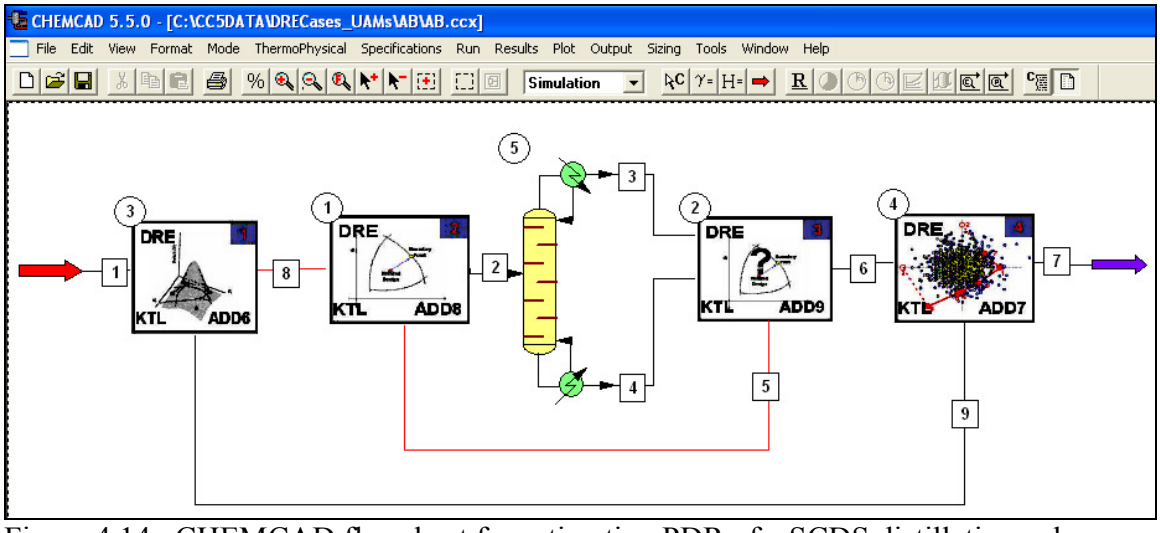


Figure 4.14. CHEMCAD flowsheet for estimating PDR of a SCDS distillation column.

The SMSD procedure coupled with CHEMCAD has the following limitations:

1. Only can be used for estimating the PDR of a SCDS binary distillation column with

one feed, one top product and one bottom product.

2. The component feed flow rates are to be the uncertain parameters with uncertainty described by independent normal distributions.
3. Only the following three process constraint specifications options are considered: 1) minimum top product purity, 2) maximum bottom product impurity, and 3) maximum component mass flow rate in bottom product.

The description of each UAM's computations follows.

4.6.1. Description of the UAM's developed for the SMSD procedure

Five types of files were created to develop each of the UAM's. Table 4.10 contains a general description of these five types of files. Instructions to create the files may be found in the CHEMCAD UAM's manual (CHEMCAD, 2007). For UAM ADD7 also a FORTRAN DLL was developed, FDLLUAM7.dll.

FDLLUAM7.dll contains the FORTRAN subroutines used by the SMSD in Chapter 3 to compute: the parameter space subdivision, the connecting planes to build the CBA, the MCI and the most significant direction. Appendix A contains a detailed description of this file. Appendix A contains also the list of files and C++ functions used for the coupling of the SMSD procedure with CHEMCAD.

The following sections present a description of the computations and dialog boxes of each of the new four modules.

Table 4.10. Description of the files required for creating a UAM.

Name form	Description
ADD*.cpp	This C++ file defines the module computations. It comes with the "USRADD.DLL" project provided by CHEMCAD and is to be customized. The CHEMCAD 5.6.4 provides ten possible UAM's: ADD1.cpp, ADD2.cpp, ADD3.cpp, ADD4.cpp, ADD5.cpp, ADD6.cpp, ADD7.cpp, ADD8.cpp, ADD9.cpp, and ADD10.cpp .
ADD*.my	This type of file defines the visual aspect of the UAM's dialog box. The dialog box is used for input/output of data to/from simulation through the module's data array. Generally, boxes with white background are used to indicate that they are to enter data and boxes with gray background to indicate the contrary, i.e. that they are used to display data. CHEMCAD's manuals refer the module's data array as dialog box variables or UAM's parameter array. The module requires as many files as the number of tabs that make up its dialog box. CHEMCAD utility program Screen Builder may be used to create this type of file.
ADD*.map	Text file that defines the dialog box data array. The file may be created using any text editor, e.g. notepad or wordpad.
$ADD*.lab	Text file that defines labels and format for the UAM dialog box's variables in a CHEMCAD. The file may be created using any text editor.
ADD*.sym	This file defines the module's icon to be used in the CHEMCAD flow sheet. CHEMCAD provides default icons that may be used for the UAM's. However the user may create new icons, as those shown in Figure 4.14 that were created for the SMSD procedure.

4.6.1.1. Module ADD6.

The dialog box for this module has the two tabs shown in Figures 4.15 and 4.16. The pictures in these figures include notes to describe the data. Table 4.11 lists the data that must be entered by the user in this module's dialog box. When the user is going to start a new computation a value of zero must be entered in the box in front of the label "iteration number". Stream and unit ID numbers are required by this and the other three UAM's to have access to units and streams' data. The ID numbers entered in this dialog box are written by this module in the dialog boxes of the other three modules.

This module controls the start of the outer loop iterations, keeps track of the outer loop iterations, and computes the axial radial directions as described in Chapter 3. The

flow chart in Figure 4.17 shows the sequence of the computations. The initial values that this module sets in modules ADD7 and ADD8 are discussed when describing those modules.

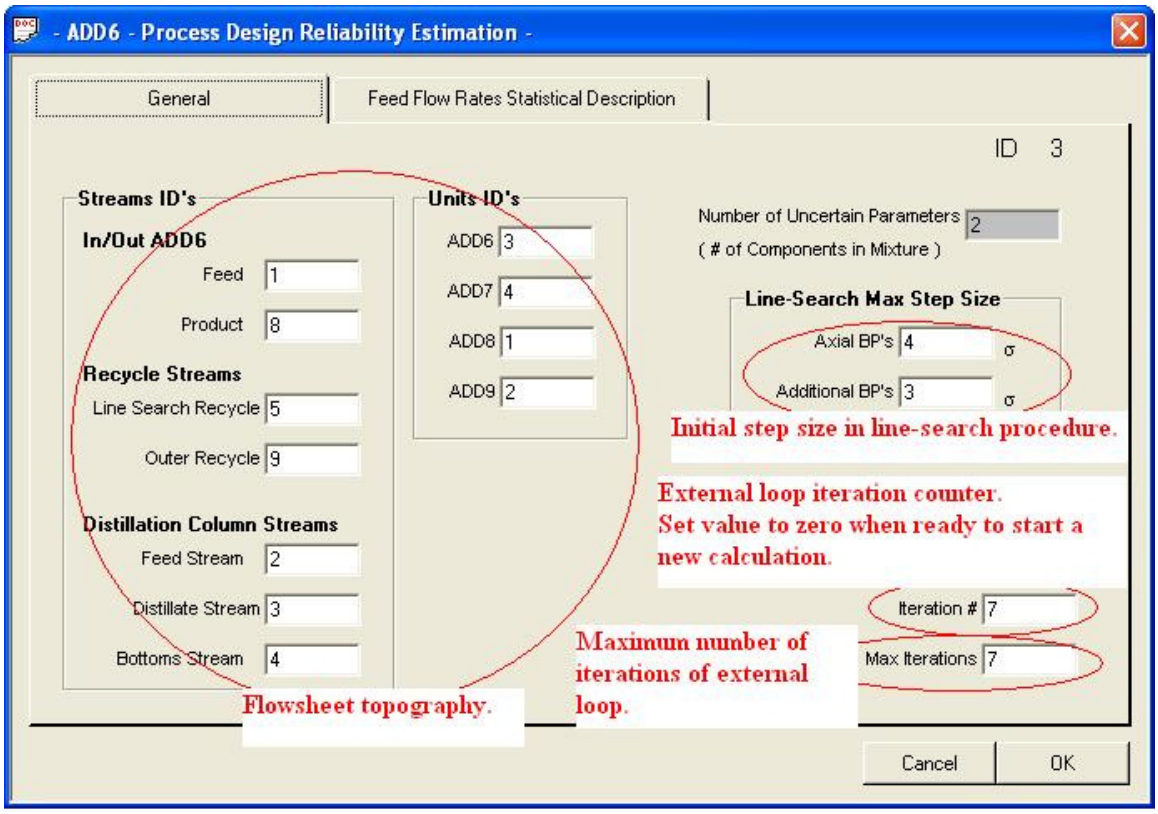


Figure 4.15. "General" tab of the module ADD6's dialog box.

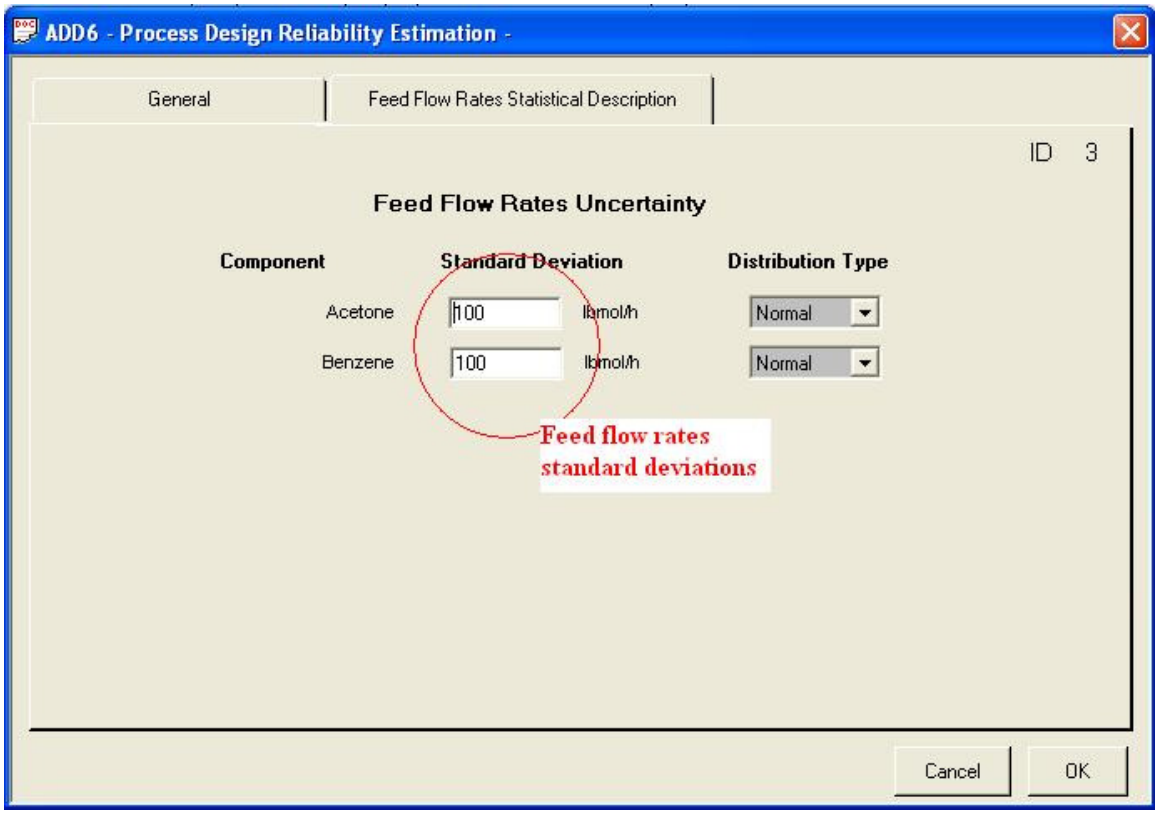


Figure 4.16. "Feed Flow Rates Statistical Description" tab of the module ADD6's dialog box.

Table 4.11. Input data for module ADD6.

Tab	Input data
"General"	Stream ID's: Feed to ADD6, product from ADD6, line-search recycle, outer recycle, feed stream to distillation column, distillate stream, bottom stream.
	Unit ID's for modules: ADD6, ADD7, ADD8, and ADD9.
	Linea-search maximum step sizes to search for: axial BP's, additional BP's.
	Iteration #.
	Maximum iterations.
"Feed Flow Rates Statistical Description"	Feed flow rate's standard deviations.

ACRONYM KEY:
DB dialog box
F "Flag" in ADD7's DB
I6 "Iteration #" in ADD6's DB
I7 "Iteration #" in ADD7's DB
NUP "Number of Uncertain Parameters" in ADD6's DB
TI6 "Max. Iterations" in ADD6's DB

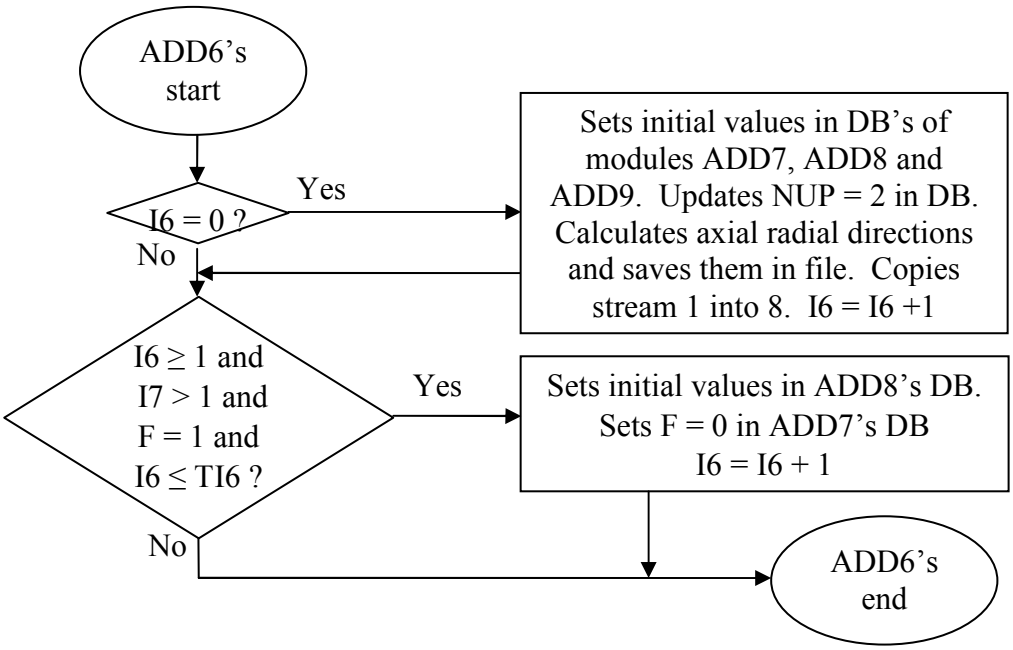


Figure 4.17. Flow chart of module ADD6's computations.

4.6.1.2. Module ADD8

Figure 4.18 shows the dialog box for this module. The only datum that must be entered by the user is the line-search procedure's maximum number of iterations. The data in gray background boxes are updated by this module, and modules ADD6 and ADD9.

In the first outer iteration of the SMSD procedure module ADD6 writes the unit ID numbers in module ADD8's dialog box. Each time an outer iteration starts module

ADD6 sets the initial values listed in Table 4.12 in module ADD8's dialog box. In this table the "Computed distance" is the scalar δ used by the line-search algorithm and described in Section 2.3.2. Its maximum value, "Maximum Dimensionless Distance", is one. The latter value is used in the first iteration of the line-search procedure.

This module computes the component feed flow rates for the distillation column in the line-search of BP's and keeps track of the inner loop iterations. Figure 4.19 shows the sequence of computations executed by this module.

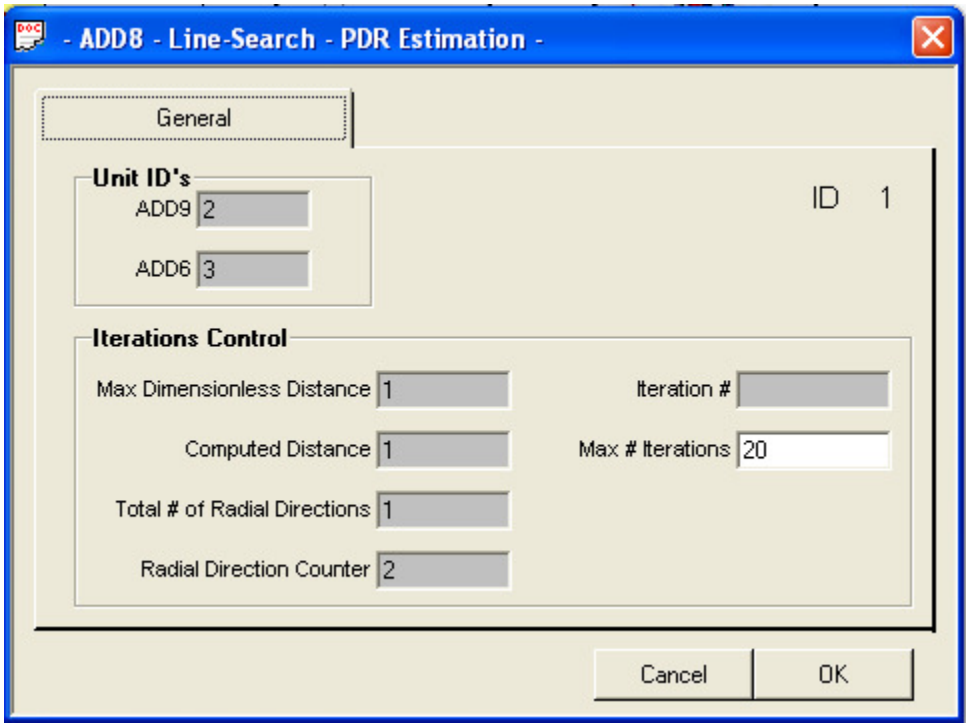


Figure 4.18. Module ADD8's dialog box.

Table 4.12. Initial values set by module ADD6 in module ADD8's dialog box.

Maximum dimensionless distance	1
Computed distance	1
Total number of radial directions	0
Radial direction counter	0
Iteration #	0

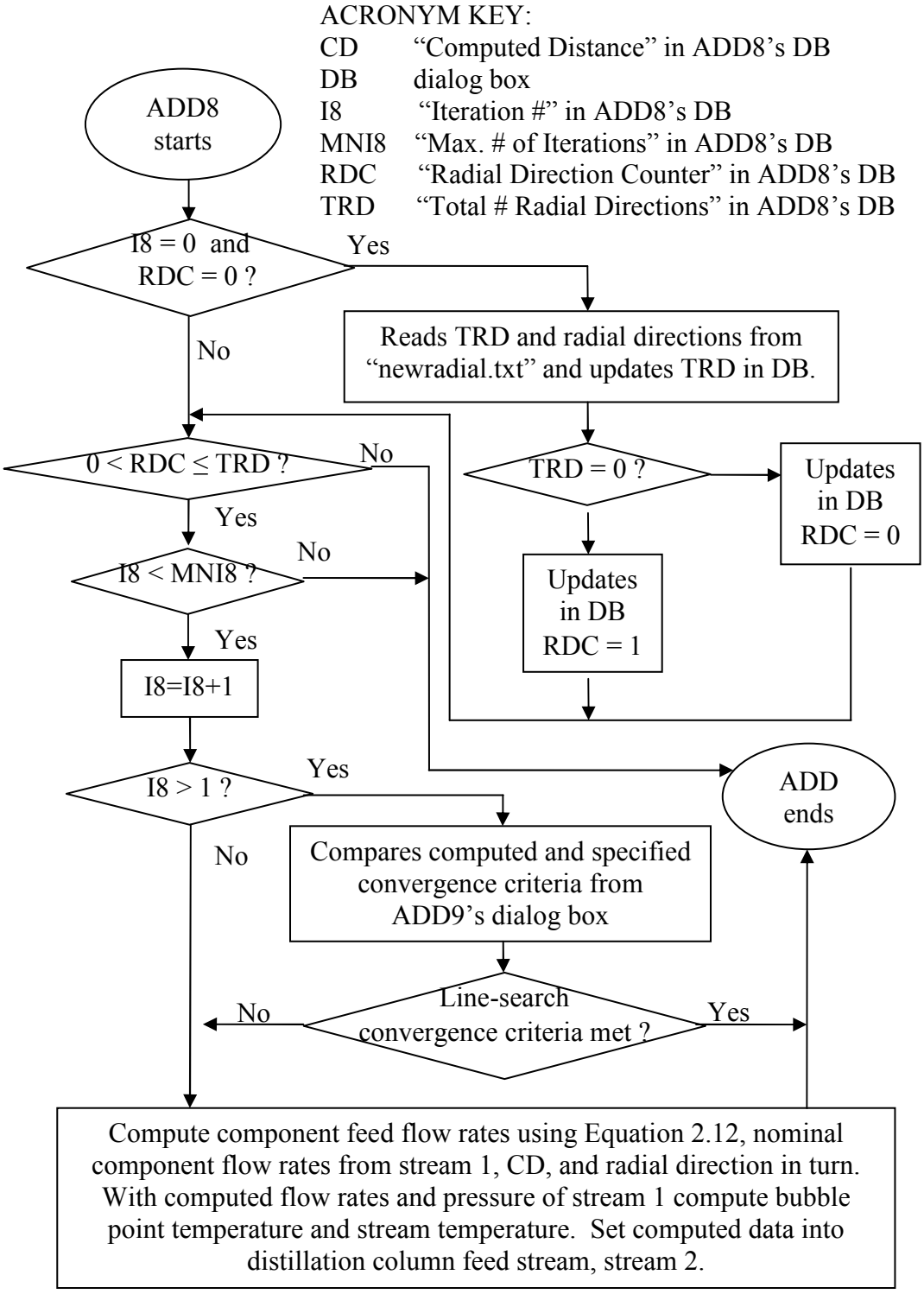


Figure 4.19. Flow chart of module ADD8's computations.

4.6.1.3. Module ADD9

This module's dialog box is shown in Figure 4.20. The input data are the process constraints and the line-search procedure convergence criteria. The user must select the process constraints from the available options: 1) component mole fraction in bottoms, 2) component mass flow rate in bottoms, and 3) component mole fraction in distillate. For the line-search convergence criteria, tests with the case studies for this development showed that a value of 1e-4 for both criteria produced sufficiently accurate BP's without requiring excessive number of MS's.

In the first iteration of the SMSD procedure, module ADD6 writes the stream and unit ID's in module ADD9's dialog box. The computed constraints and convergence criteria shown in the gray background boxes are computed and updated by this module.

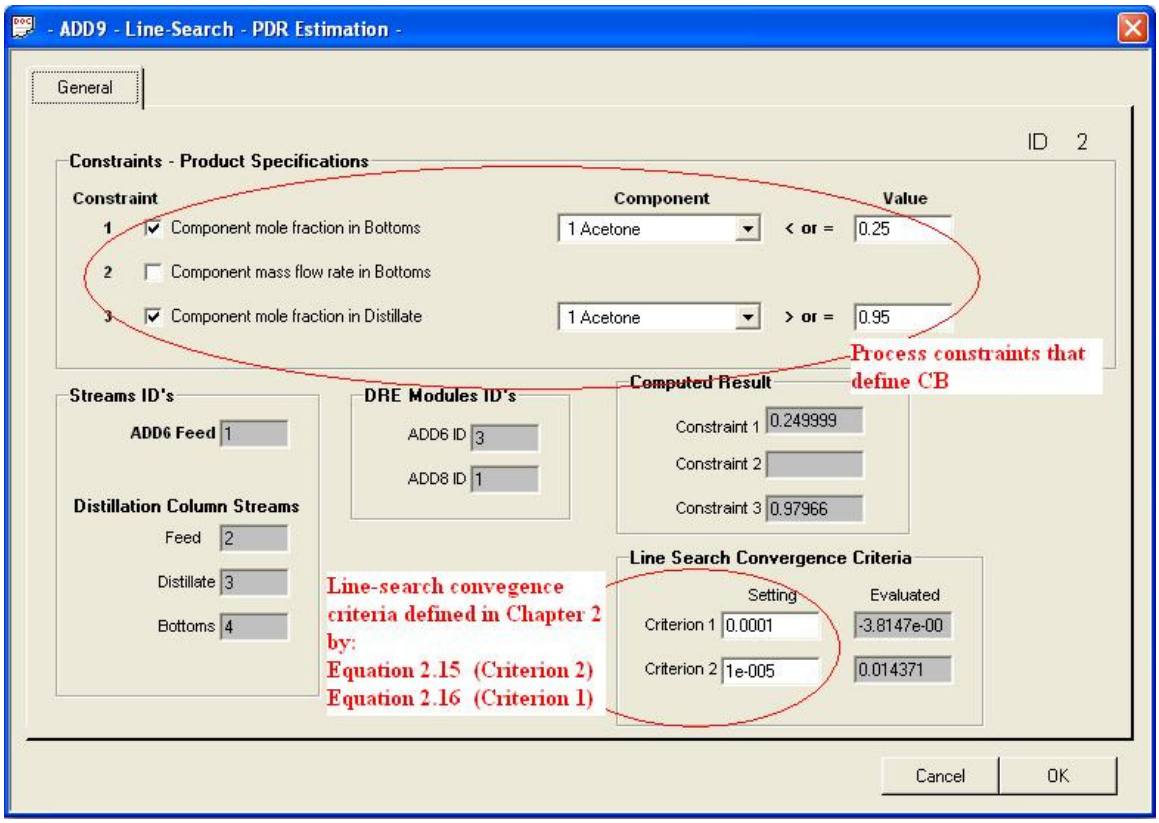


Figure 4.20. Module ADD9's dialog box.

This module uses the SCDS distillation column simulation results to evaluate the process constraint equations and convergence criteria. When the line-search procedure has not converged, it computes a new value for the line-search scalar, as described in Section 3.2, and updates this value in module ADD8's dialog box. Also, based on the computed convergence criteria, this module updates the inner recycle stream data and data in module ADD8's dialog box as indicated in the flow chart shown in Figure 4.21.

This module saves results from the line-procedure in two files. In addition to saving results in file "newBP.txt", this module saves the line-search procedure's iterative results in a file named "resadd9.txt". This file is created for debugging purposes, but it is not used by subsequent computations.

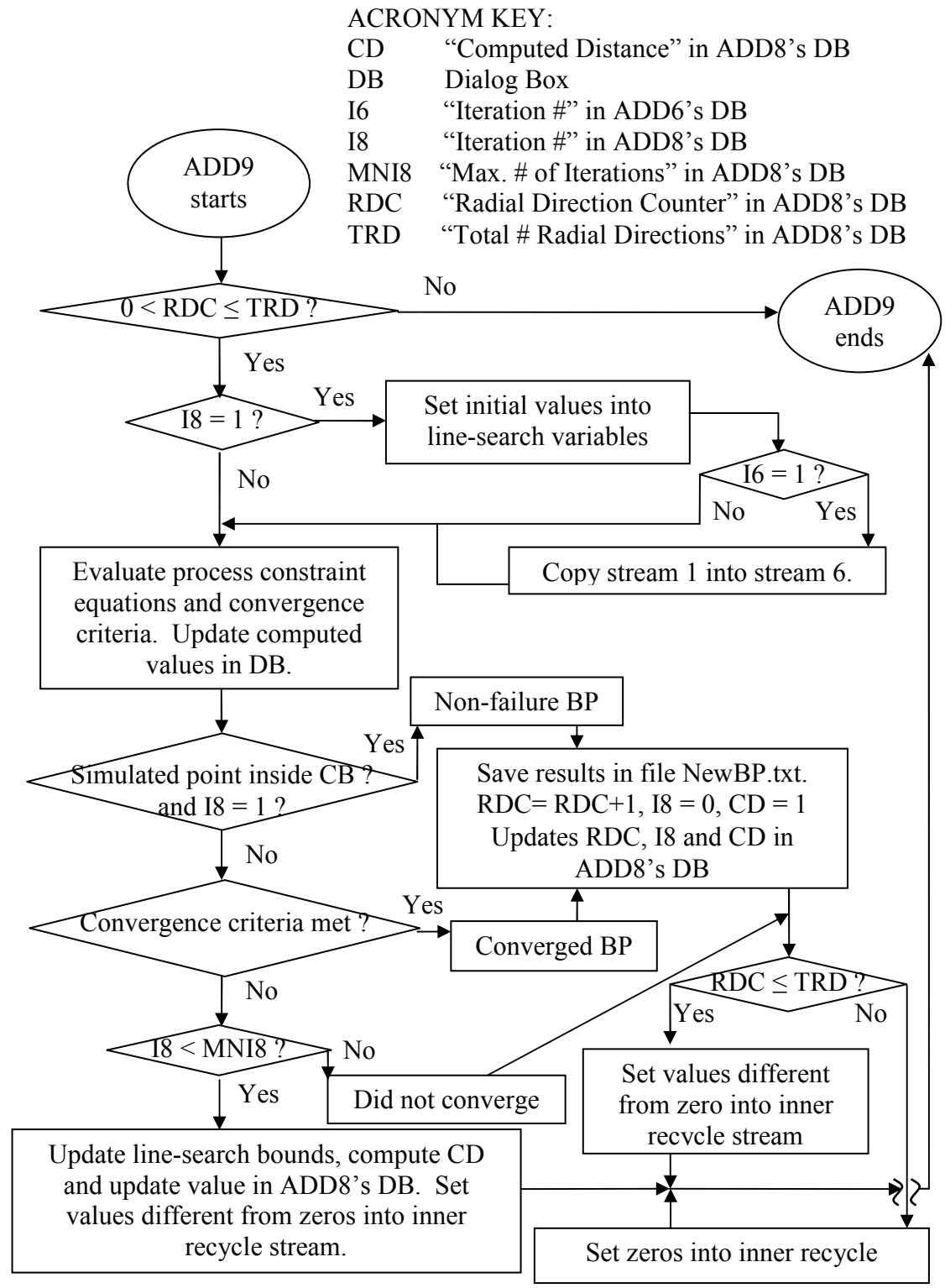


Figure 4.21. Flow chart with module ADD9's computations.

4.6.1.4. Module ADD7

This module's dialog box is illustrated in Figure 4.22. The user must enter the number of MC sets and the criteria for the SMSD procedure's convergence. Tests conducted in Chapter 3 showed that a value of 10 for criterion 1 and a value of 1 for criterion 2 produced sufficiently accurate PDR estimates without requiring an excessive number of additional BP's.

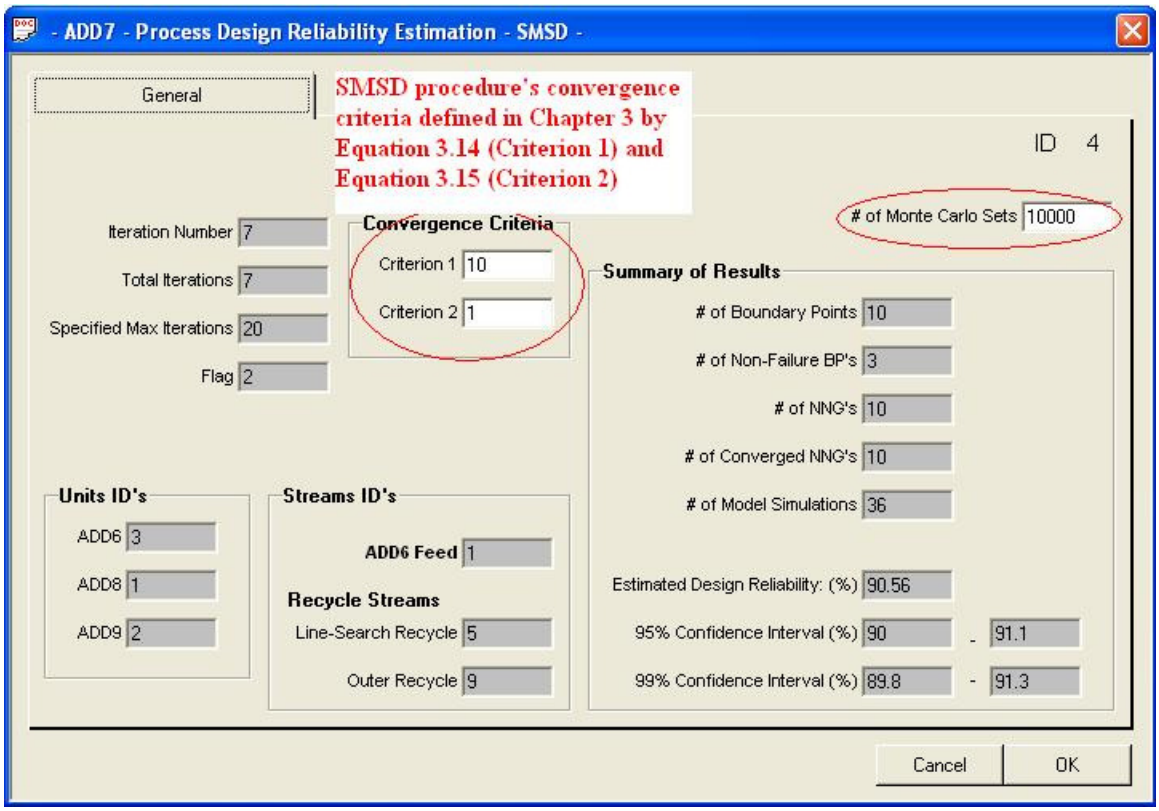


Figure 4.22. Module ADD7's dialog box.

In the first iteration of the SMSD procedure, module ADD6 writes the stream and unit ID's in module ADD7's dialog box. Also in the first iteration of the SMSD procedure module ADD6 writes the initial values listed in Table 4.13 in module ADD7's dialog box. Every time a new outer iteration is going to start module ADD6 updates the value in front of the label "Flag" to zero to signal that the inner loop is searching for a

BP. The MCI results are updated in the dialog box each time the module gets those results.

Table 4.13. Initial values set by module ADD6 in module ADD7's dialog box.

Iteration number	1
Total iterations	Max. iterations in module ADD6's dialog box
Specified max. iterations	Max. iterations in module ADD6's dialog box
Flag	0

This module computes the parameter space subdivision as described in Section 2.3.1, and the CBA and the MCI as described in Section 3.3. For subsequent iterations, the module adds the BP and updates the CBA and MCI as also explained in Section 3.3. This module also evaluates the SMSD procedure's convergence criteria. When the convergence criteria have not been met, the module sets new values for the outer recycle stream information to signal CHEMCAD that a new iteration of the outer loop will be required. Then the module computes the statistically most significant direction as described in Section 3.3. When the convergence criteria have been met, the module signals the end of the computations by setting the outer recycle stream's variables to zero and a value 2 in the box in front of the label "Flag" in the dialog box. The flow chart in Figure 4.23 shows the sequence of the computations. In addition to displaying the MCI results in the dialog box, this module also saves them in a file named "BoundaryInfo.txt".

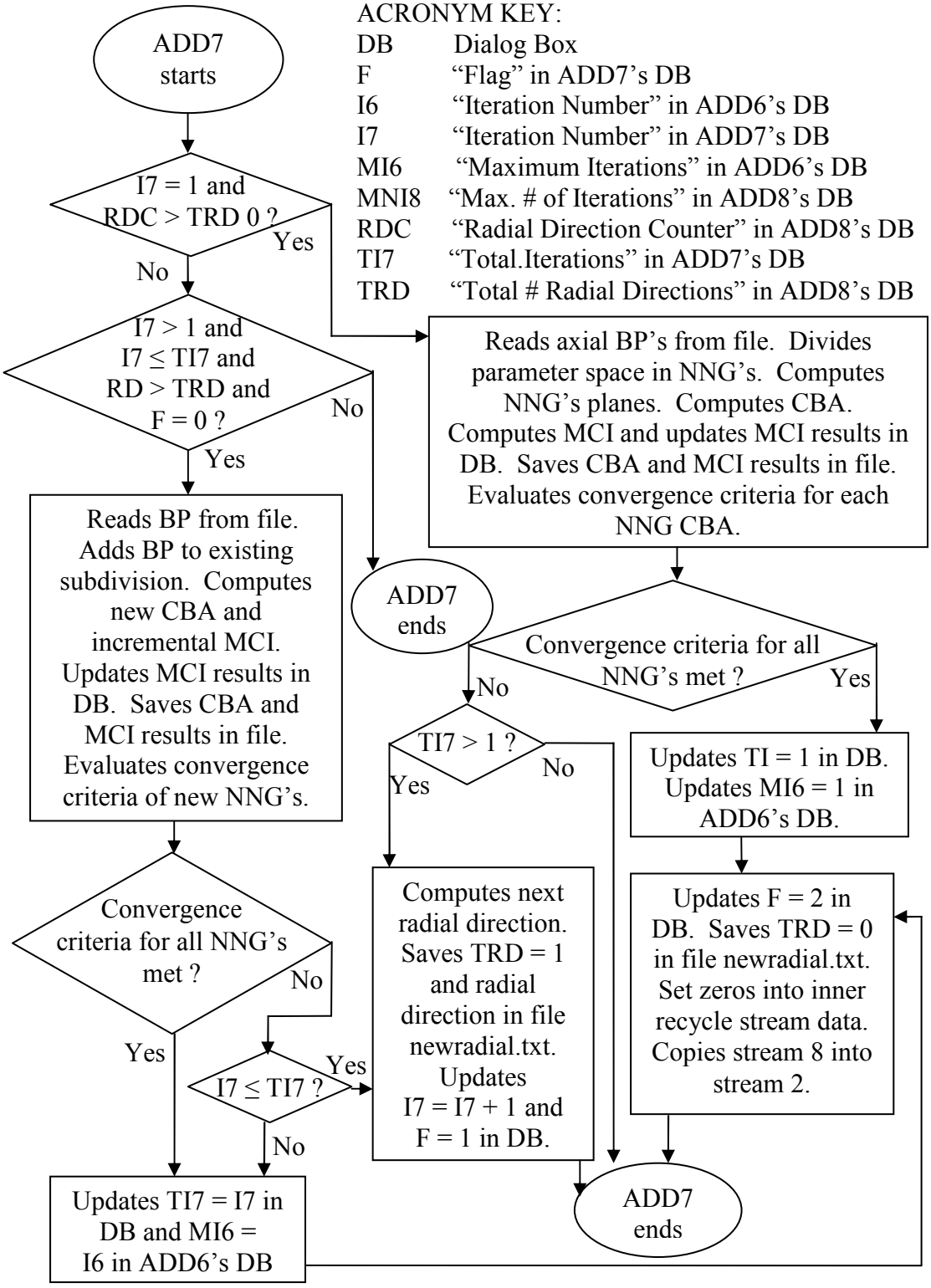


Figure 4.23. Flow chart with module ADD7's computations.

4.6.2. Setting up a flow sheet to estimate PDR by SMSD procedure

Before starting a design reliability calculation using the SMSD procedure linked to CHEMCAD, the user must have the DLL that contains the modules' executable code, USRADD.DLL, in the CHEMCAD directory CC5. Also the FORTRAN DLL, FDLLUAM7.dll, must be in the same directory. For constructing a new flow sheet that contains the symbols shown in Figure 4.14 for modules ADD6, ADD7, ADD8 and ADD9, the user must install the symbols as described in the CHEMCAD help. The two DLL's and symbol files are provided on the attached CD.

The easiest way to start a PDR calculation with the SMSD procedure coupled with CHEMCAD is by using as starting point a copy of the CHEMCAD job directory of a previous case calculation. Then proceed to modify the component list, stream 1's data and each module's dialog boxes' data, including that of the SCDS unit. The other option is to start by creating a new CHEMCAD job and setting up a flow sheet in the traditional way that looks like the one shown in Figure 4.14.

Figures 4.15, 4.16, 4.18, 4.20 and 4.22 show the modules' dialog boxes with the data for the A/B design case described in Section 4.5.2 to compute the PDR by the CMCI procedure. However here only the component feed flow rates are the uncertain parameters, while in Section 4.5.2 tray efficiency and BIP's are also uncertain parameters. For this example a maximum number of iterations of twenty was initially set in module ADD6's dialog box. However the procedure only required seven iterations. The input data for the SCDS unit, with exception of the condenser and reboiler specifications, correspond to the list in Table 4.2. The condenser and reboiler specifications are listed in Table 4.4 as the condenser and reboiler control variables.

After all the input data have been entered in the modules' dialog boxes the user may run the CHEMCAD simulation in the following order. First only run a simulation of the first module, module ADD6. This is necessary for the module to prepare to execute the iterative and sequential computations until convergence or the predefined maximum number of iterations. When CHEMCAD signals that the module ADD6 simulation is finished, then the user may run the whole flow sheet simulation. The results from the SMSD calculation can be read from the module ADD7's dialog box or from the file BondaryInfo.txt located in the CHEMCAD job directory. The file includes computing times.

4.6.3. Case studies and results

The performance of the SMSD procedure coupled with CHEMCAD was evaluated by comparing the results obtained with this method and the CMCI procedure coupled with CHEMCAD for three designs. PDR estimates, MS's and computation time are compared. The three binary distillation designs with component feed flow rates as uncertain parameters described in Table 2.1 were used for testing. The modification in the design specification for the A/B and M/I designs described in Section 4.5.3 was also required here.

Based on the comments in Section 4.6.1, for the three case studies a value of 1E-4 for the two line-search's convergence criteria was set. The maximum initial step for the search of axial BP's was 4 and for the search of additional BP's was 3, as in Chapter 3. Also as in Chapter 3, the SMSD procedure's convergence criteria, criterion 1 and criterion 2 in Figure 19, were c_1 = 10.0% and c_2 = 1.0%, respectively.

A summary of the PDR estimates, MS's and computing time is presented in Table 4.14. This table includes the PDR estimates obtained by the CMCI procedure using two sizes of CMCI sets. For the SMSD procedure, the PDR's estimates obtained in the first iteration and at convergence are included. The results are in agreement with the results obtained in Chapter 3. The SMSD procedure requires two to three orders of magnitude less computing time and fewer MS's than CMCI does to converge to equally accurate estimates.

Table 4.14. PDR estimates obtained with CMCI and SMSD procedures coupled with CHEMCAD.

		CMCI[a]		CMCI[b]		SMSD[b,c]			SMSD[d]			
Mixture	*p*	PDR (%)	Time (s)	PDR (%)	Time (s)	PDR (%)	MS's	Time (s)	PDR (%)	BP's	MS's	Time (s)
A/B	2	90	55	91	524	86	10	< 1	91	10	36	< 2
A/W	2	93	50	93	406	88	9	< 1	93	10	41	< 1
M/I	2	98	278	98	2808	95	11	< 1	98	10	50	< 4

[a] 1,000 MC sets.
[b] 10,000 MC sets.
[c] At initialization, i.e. with only the four axial BP's.
[d] At convergence.

4.7. OPT procedure coupled with CHEMCAD

VB code for coupling the OPT procedure with CHEMCAD was written in the EXCEL/VBA environment of the same EXCEL file used for coupling the CMCI procedure with CHEMCAD. As for the coupling of the CMCI procedure, the code was organized in VB subroutines and controlled by a main subroutine.

Also for this development a CHEMCAD job with a flowsheet containing a CHEMCAD SCDS distillation column with one feed stream, one top product stream and one bottom stream is necessary.

A description of the code's computations follows. Description of the input data, results, and instructions to set up a calculation and run the procedure are included and explained through an example.

4.7.1. Description of the OPT procedure's VB code computations

The OPT procedure's calculations are those described in Chapter 2 with the following modifications to improve the computational efficiency of the procedure.

1. The line-search procedure uses the modifications described in Section 3.3 for the SMSD procedure.
2. To reduce the underestimation of the CB by the connecting plane in open ended NNG's the procedure does the following. Once the procedure determines that a NNG has only non-failure BP's, then the procedure assumes that all the MC sets in that NNG fall inside the CB.
3. For designs with more than two uncertain parameters new criteria for establishing the convergence of the OPT procedure were used. If a NNG has only non-failure BP's then it is assumed that all the NNG's statistical significant parameter space is inside the CB and no further computations are required for that NNG. When a new BP is added, p new NNG's are created and new CBA's are built for those NNG's. Incremental MCI is computed to get updated PDR estimates. If the tangential estimate does not change significantly with respect to its previous value then it is assumed that no further computations for the recently added NNG's are required. In terms of an equation it is:

$$\left| \hat{\Re}^T \Big|^{new} - \hat{\Re}^T \Big|^{old} \right| \leq \varepsilon_T \qquad (4.1)$$

A main VB subroutine was programmed to execute the OPT procedure's sequential and iterative computations outlined in the flowchart in Figure 2.6. The OPT procedure's code uses the five subroutines described in Table 4.1 for activating the connection with the CHEMCAD job and reading input data from the EXCEL file and CHEMCAD job.

Appendix A includes a list with description of the VB subroutines written for the computations of the linear-search procedure, the parameter space subdivision, the initial and updated CBA's, the initial and incremental MCI, the convergence criteria evaluation, and the selection of the next radial direction. The line-search procedure subroutine uses the CHEMCAD job to run the distillation model simulation required in the search of BP's.

As the CMCI procedure coupled with CHEMCAD, the OPT procedure coupled with CHEMCAD reads the MC sets required for the MCI from the worksheet "MCPoints". Therefore the user must update the MC sets for the specific problem in turn. The user may use the subroutines described in Section 4.5.2 to generate the MC sets.

The limitations of the OPT procedure coupled with CHEMCAD are the same as those described in Section 4.5.1. In addition the current code is limited to a maximum of 200 BP's and/or 2000 NNG's, whichever occurs first. These values may be modified. However they are restricted by the EXCEL limitation of array sizes and/or computer limitations of RAM memory.

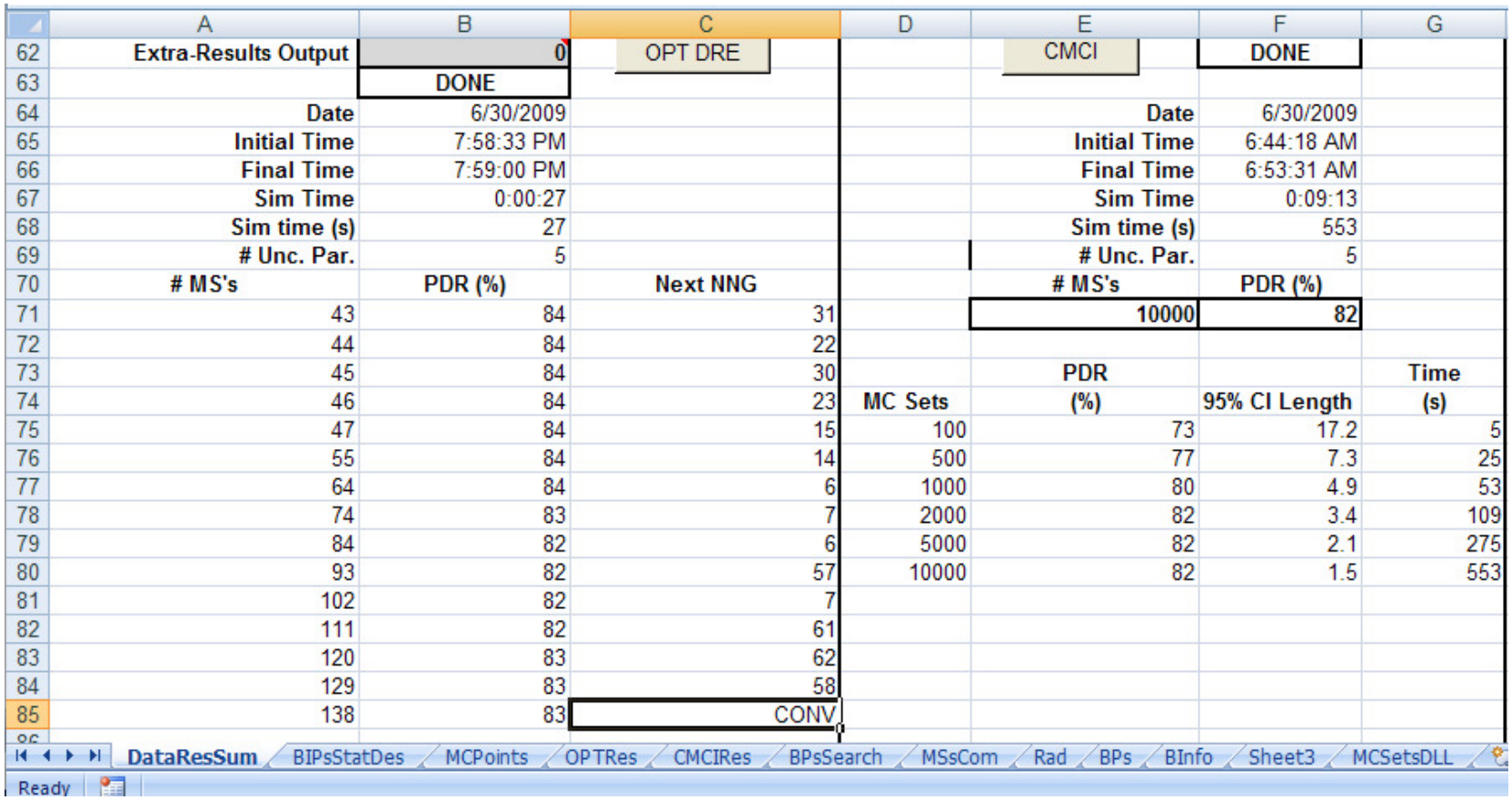
4.7.2. Input data set up and calculation example

Consider the same example described in Section 4.5.2. For the OPT procedure coupled with CHEMCAD, steps one through five described in Section 4.5.2 may be

followed. Then the user must choose the calculation options for the OPT procedure. The left side of the screen shot shown in Figure 4.9 shows the area of the worksheet where the calculation options must be selected.

As for the CMCI procedure, it is recommended to select the option to run again steps one through four. From the tests with the case studies presented in Chapter 2 and 3, it was determined that an initial step size of three in the line-search procedure was adequate for reducing unnecessary MS's without affecting the accuracy of the CBA. Also it was found that 10,000 MC sets were sufficient for an accurate performance of the OPT procedure. It is recommended to not select writing extra-results from the calculations to reduce the computation time, unless those results are needed. The extra-results include the distribution of MC sets for each NNG after each MCI. These results may be useful for debugging. After the data in the gray background boxes have been entered the user may run the procedure by clicking the button with the label "OPT DRE".

Figure 4.24 shows a screen shot of the worksheet "DataResSum" where the summary of results of the OPT procedure were written. The summary includes computing time, used MS's and the list of next NNG's where the search of new BP's was conducted. Figures 4.25 shows a screen shot with the OPT procedure results written on worksheet "OPTRes". The results presented here include the PDR estimates with each CBA and the 95% CI for the tangential PDR estimate. Also it includes the final distribution of MC sets in each NNG.



	A	B	C	D	E	F	G
62	Extra-Results Output	0	OPT DRE		CMCI	DONE	
63		DONE					
64	Date	6/30/2009			Date	6/30/2009	
65	Initial Time	7:58:33 PM			Initial Time	6:44:18 AM	
66	Final Time	7:59:00 PM			Final Time	6:53:31 AM	
67	Sim Time	0:00:27			Sim Time	0:09:13	
68	Sim time (s)	27			Sim time (s)	553	
69	# Unc. Par.	5			# Unc. Par.	5	
70	# MS's	PDR (%)	Next NNG		# MS's	PDR (%)	
71	43	84	31		10000	82	
72	44	84	22				
73	45	84	30		PDR		Time
74	46	84	23	MC Sets	(%)	95% CI Length	(s)
75	47	84	15	100	73	17.2	5
76	55	84	14	500	77	7.3	25
77	64	84	6	1000	80	4.9	53
78	74	83	7	2000	82	3.4	109
79	84	82	6	5000	82	2.1	275
80	93	82	57	10000	82	1.5	553
81	102	82	7				
82	111	82	61				
83	120	83	62				
84	129	83	58				
85	138	83	CONV				

Figure 4.24. Screen shot from worksheet "DataResSum" showing on the left side the OPT procedure's summary of results.

	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB
3			NumMSs	NumMSs																	
4	NumPts	NumNNG's	noTanEval	Total	Tan	Opt	Pess	Tan 95%CIT	Tan 95%CIT	Pess 95%CIT	Pess 95%CIT	Time	Sim Time(s)	Old NNG	NNG	neightot	failtan	passfail	failfail	bapprox	
5	10	32	23	43	84	84	13	83.35	84.78	12.04	13.35	7:58:37 PM	4		1	0	0	0	0	1	
6	11	36	24	44	84	84	15	83.35	84.78	13.89	15.28	7:58:38 PM	1	31	2	9	2	2	2	1	
7	12	40	25	45	84	84	18	83.35	84.78	17.32	18.83	7:58:39 PM	1	22	3	10	1	6	1	1	
8	13	44	26	46	84	84	20	83.35	84.78	19.21	20.78	7:58:41 PM	2	30	4	1	0	0	0	1	
9	14	48	27	47	84	84	23	83.35	84.78	22.33	23.99	7:58:42 PM	1	23	5	44	14	13	14	1	
10	15	52	30	55	84	84	25	83.33	84.76	24.04	25.74	7:58:44 PM	2	15	6	56	9	35	9	1	
11	16	56	34	64	84	84	26	83.28	84.72	25.63	27.36	7:58:46 PM	2	14	7	53	13	27	13	1	
12	17	60	39	74	83	83	28	82.57	84.03	26.71	28.46	7:58:47 PM	1	6	8	56	13	25	13	1	
13	18	64	44	84	82	82	29	81.61	83.10	27.72	29.49	7:58:49 PM	2	7	9	1	0	1	0	1	
14	19	68	48	93	82	82	29	81.60	83.09	28.05	29.83	7:58:51 PM	2	6	10	5	0	5	0	1	
15	20	72	52	102	82	82	29	81.71	83.20	28.37	30.15	7:58:53 PM	2	57	11	6	3	2	3	1	
16	21	76	56	111	82	82	30	81.63	83.12	28.63	30.42	7:58:55 PM	2	7	12	0	0	0	0	1	
17	22	80	60	120	83	83	30	81.76	83.25	28.87	30.66	7:58:57 PM	2	61	13	46	3	30	3	1	
18	23	84	64	129	83	83	30	81.92	83.40	29.21	31.01	7:58:58 PM	1	62	14	271	27	188	27	1	
19	24	88	68	138	83	83	30	81.96	83.44	29.58	31.38	7:59:00 PM	2	58	15	263	32	190	32	1	
20															16	44	3	31	3	1	
21															17	1	0	0	0	1	
22															18	9	0	5	0	1	
23															19	9	0	5	0	1	
24															20	2	0	0	0	1	
25															21	48	0	25	0	1	
26															22	309	2	213	2	1	
27															23	288	1	211	1	1	
28															24	45	0	0	0	1	
29															25	0	0	0	0	1	
30															26	3	0	1	0	1	

DataResSum | BIPsStatDes | MCPoints | **OPTRes** | CMCIRes | BPsSearch | MSsCom | Rad | BPs | BInfo | Sheet3 | MCSetsDLL

Figure 4.25. Screen shot from worksheet “OPTRes” showing OPT procedure results.

4.7.3. Case studies and results

The OPT procedure performance is evaluated by estimating the PDR for the binary and ternary distillation column designs described in Table 2.1. As described in Section 4.5.3 reboiler heat duty instead of reboiler vapor was used as design specification for the A/B, M/I and Acetone/Benzene/Toluene (A/B/T) designs. Table 4.1 contains the reboiler heat duty specified for the A/B and M/I designs. For the A/B/T mixture the reboiler heat duty value is 1.9E6 Btu/h.

First, the M/I design with two uncertain parameters is used to analyze the accuracy of BP's and tangents evaluated by the line-search procedure and the CHEMCAD distillation unit. This analysis is similar to that presented in Chapter 3 for the OPT procedure using the stand alone FORTRAN distillation model. Later the performance of the OPT procedure coupled with CHEMCAD is tested with all the designs.

The CB of the M/I design with two uncertain parameters is open-ended. This is illustrated in Figures 3.8 and 3.9 using the results from the CMCI procedure. The initial CBA has only one actual axial BP in the positive direction of the 2-methyl-1-butene feed flow rate with respect to the nominal design. In the other axial directions there are non-failure BP's. The search for the only axial BP is used for the evaluation of the procedure's performance. The initial PDR was estimated twice using different initial step sizes in the line-search procedure. The step sizes were computed using $M = 3$ and $M = 4$, i.e. three and four times the component feed flow rate's standard deviation. The convergence criteria for the line-search procedure were ε_δ = 1E-5 and ε_g = 1E-4. These convergence criteria settings produced accurate BP's without requiring excessive MS's. Figure 4.26 shows that the procedure converged to approximately the same axial BP with

both initial step sizes. Figure 4.27 shows the computed axial BP's and tangents in the component feed flow rate parameter space. No significant difference in the computed values is observed.

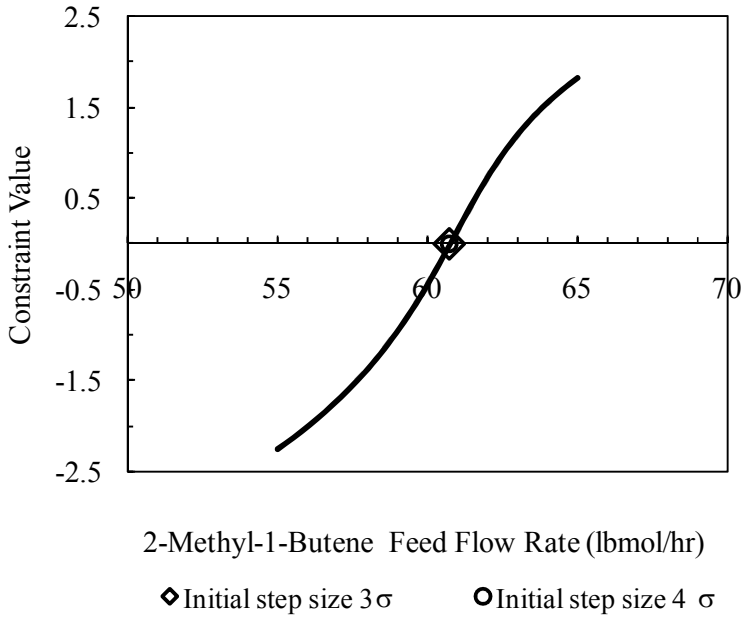


Figure 4.26. Constraint boundary as a function of the 2-methyl-1-butene feed flow rate and BP's found with the OPT procedure coupled with CHEMCAD when initial step sizes of three and four times the component feed flow rate's standard deviation.

Then the OPT procedure was run to convergence with $\varepsilon_{OP} \leq 1\%$ as defined in Equation 2.28 and using 10,000 MC sets as in Chapter 3. For the search of additional BP's the initial step size was the same as the one used for the search of axial BP's. Table 4.15 shows the PDR estimates obtained. The accuracy of the initial tangential PDR estimates for the two options is the same. Both options required the same number of BP's to converge. However when using M = 4 more MS's were required because the line-search procedure requires a few more iterations per BP. The OPT procedure coupled with CHEMCAD required fewer MS's than the OPT procedure using the stand-alone

FORTRAN distillation model simulator. The results for the latter are presented in Tables 3.11 and 3.12.

In summary the OPT procedure coupled with CHEMCAD was more computationally efficient than OPT procedure using the stand alone FORTRAN distillation model.

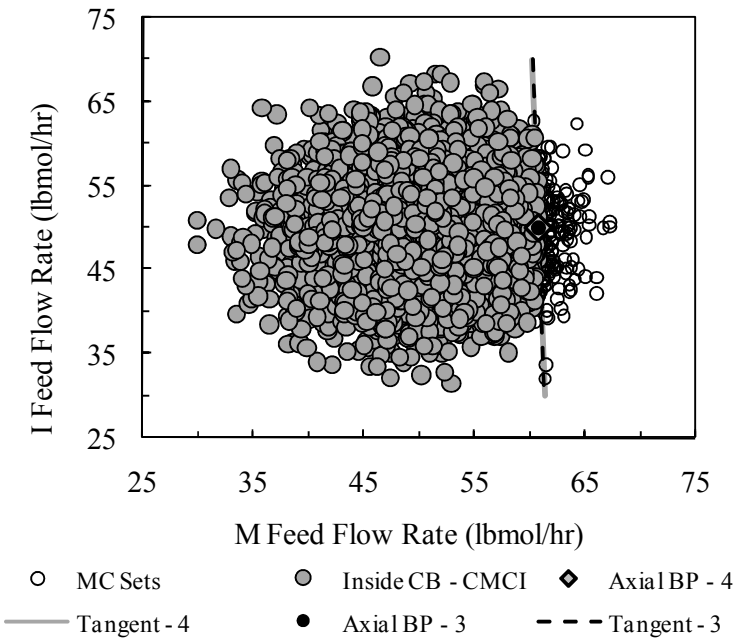


Figure 4.27. Results of the CMCI procedure coupled with CHEMCAD for the M/I design with two uncertain parameters. Also axial BP's and tangents computed by the OPT procedure coupled with CHEMCAD are shown. Results when using three and four times the component feed flow rate's standard deviation are shown.

Table 4.15. PDR estimates for the M/I design with two uncertain parameters obtained by the OPT procedure coupled with CHEMCAD.

	using 3 σ				using 4 σ			
BP's	MS's	TDRE (%)	ODRE (%)	PDRE (%)	MS's	TDRE (%)	ODRE (%)	PDRE (%)
4	13	98	98	93	15	98	98	95
5	24	98	98	95	23	98	98	97
6	25	98	98	98	32	98	98	98

Next the PDR's of the designs described in Table 2.1 were estimated. 10,000 MC sets were used as in Chapter 3. The initial step size in the line- search procedure was computed using $M = 3$. The line-search procedure's convergence criteria were ε_δ = 1E-5 and ε_g = 1E-4. For the designs with two uncertain parameters the OPT procedure's convergence criterion defined by Equation 2.28 was used with $\varepsilon_{OP} \leq 1\%$. For designs with more than two uncertain parameters the OPT procedure's convergence is evaluated as described in Section 4.6.1 with $\varepsilon_T \leq 0.2\%$. A maximum of thirty iterations was set, i.e. no more than 29 additional BP's were allowed.

Table 4.16 shows the initial PDR estimates obtained by the OPT procedure coupled with CHEMCAD and the CMCI PDR estimates obtained with 10,000 MC sets. With the exception of the A/B designs with three and five uncertain parameters the initial PDR estimates evaluated by the OPT procedure are within 1% of error with respect to the CMCI PDR estimates.

Table 4.17 shows the initial errors in the PDR estimates with respect the CMCI PDR estimates obtained with the OPT procedure coupled with CHEMCAD and the OPT procedure using the stand alone FORTRAN distillation model simulator. The errors for the OPT procedure using the stand alone FORTRAN distillation model simulator were computed using the results shown in Tables 2.7 and 2.8. For the designs considered in this table the initial accuracy of the OPT procedure coupled with CHEMCAD is better than that of the OPT procedure using the FORTRAN distillation model simulator. This may be attributed to more accurate BP's and tangents being computed by the procedure coupled with the CHEMCAD than the procedure using the stand alone FORTRAN distillation model simulator.

Table 4.16. PDR estimates from CMCI and OPT procedures coupled with CHEMCAD. OPT PDR estimates at initialization.

Mixture	*p*	OPT						CMCI PDR (%)
		BP's	NNG's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	
A/B	2[a]	4	4	16	90	90	83	91
A/B	3[b]	6	8	20	84	84	51	81
A/B	5[c]	10	32	43	84	84	13	82
A/W	2[a]	4	4	10	93	93	86	93
A/W	3[b]	6	8	21	69	69	31	68
A/W	5[c]	10	32	29	68	68	11	68
M/I	2[a]	4	4	13	98	98	93	98
M/I	3[b]	6	8	16	97	97	70	97
M/I	5[c]	10	32	85	82	82	1	81
A/B/T	3[a]	6	8	6	100	100	100	100
A/ B/T	4[b]	8	16	8	100	100	100	100
A/B/T	10[c]	20	1024	20	100	100	100	100

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and BPI's.

Table 4.17. Errors in initial Tangential OPT PDR estimates with respect to CMCI PDR estimates.

Mixture	*p*	BP's	OPT with stand alone model simulator		OPT coupled with CHEMCAD	
			MS's	% Error	MS's	% Error
A/B	2[a]	4	22	-0.6	16	0.8
A/B	3[b]	6	26	3.9	20	-3.5
A/B	5[c]	10	42	7.5	43	-3.0
A/W	2[a]	4	10	0.2	10	0.0
A/W	3[b]	6	20	0.1	21	-0.4
A/W	5[c]	10	28	0.1	29	-0.3
M/I	2[a]	4	16	-20.2	13	-0.1
M/I	3[b]	6	19	-7.5	16	-0.3
M/I	5[c]	10	89	-0.1	85	-0.4
A/B/T	3[a]	6	6	0.0	6	0.0
A/ B/T	4[b]	8	8	1.0	8	-0.4
A/B/T	10[c]	20	20	1.0	20	-0.4

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and BIP's.

Table 4.18 shows the PDR estimates at convergence of the OPT procedure coupled with CHEMCAD. The procedure met the convergence criteria for all the designs except the M/I design with five uncertain parameters. Note that even though the procedure did not meet the convergence criteria within the allowed number of additional BP's for the latter design, the error in the final tangential estimate with respect to the CMCI estimate is zero. For all the case studies the final tangential estimates are within 1.3% of error with respect to the CMCI PDR estimates. The OPT procedure computes accurate PDR estimates using two to three orders of magnitude less MS's than the CMCI procedure.

Table 4.18. PDR estimates from CMCI and OPT procedures coupled with CHEMCAD. OPT's estimates at convergence or maximum number of allowed iterations.

Mixture	*p*	OPT						CMCI PDR (%)
		BP's	NNG's	MS's	TPDR (%)	OPDR (%)	PPDR (%)	
A/B	2[a]	6	6	24	90	90	89	91
A/B	3[b]	11	18	48	82	82	69	81
A/B	5[c]	24	88	138	83	83	30	82
A/W	2[a]	6	6	25	93	93	93	93
A/W	3[b]	10	16	40	68	68	51	68
A/W	5[c]	18	64	77	68	68	26	68
M/I	2[a]	6	6	25	98	98	98	98
M/I	3[b]	8	12	18	97	97	89	97
M/I[d]	5[c]	39	148	290	81	81	16	81
A/B/T	3[a]	6	8	6	100	100	100	100
A/ B/T	4[b]	8	16	8	100	100	100	100
A/B/T	10[c]	20	1024	20	100	100	100	100

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and BPI's.
[d] Reached maximum number of iterations but not the convergence criteria.

Table 4.19 shows a summary of the initial and final tangential OPT PDR estimates including the estimates' 95% CI and the computing time. The change in the tangential estimates is relatively insignificant. However for some cases the time required for

convergence may be up to ten times the initial computing time. For the case studies considered here the initial tangential estimates are sufficiently accurate, but that may not be the case for other designs. Addition of BP's is normally necessary to confirm the accuracy and/or convergence of the tangential PDR estimates. Nonetheless the addition of BP's may considerably effect the OPT procedure's computational efficiency. Two things that may be considered to reduce the number of additional BP's are: 1) the improvement of the pessimistic CBA approach to reduce the uncertainty in the PDR estimates, and 2) the development of an efficient procedure to evaluate the convergence of the procedure. Improvement in the line-search procedure to reduce the number of MS's required per BP may help to maintain the OPT procedure's efficiency as BP's are added.

Table 4.19. Initial and final tangential PDR estimates from OPT procedures coupled with CHEMCAD.

Mixture	*p*	Initial				Final			
		MS's	TPDR (%)	95% CI	Time (s)	MS's	TPDR (%)	95% CI	Time (s)
A/B	2[a]	16	90	89 - 91	2	24	90	89 - 91	3
A/B	3[b]	20	84	83 - 85	3	48	82	82 - 83	31
A/B	5[c]	43	84	83 - 85	3	138	83	82 - 83	30
A/W	2[a]	10	93	93 - 94	1	25	93	93 - 94	3
A/W	3[b]	21	69	68 - 69	2	40	68	67 - 69	6
A/W	5[c]	29	68	67 - 69	3	77	68	67 - 69	15
M/I	2[a]	13	98	98 - 99	3	25	98	98 - 99	18
M/I	3[b]	16	97	97 - 97	4	18	97	97 - 97	7
M/I	5[c]	85	82	81 - 82	19	290	81	81 - 82	114
A/B/T	3[a]	6	100	100 - 100	1	6	100	100 - 100	1
A/ B/T	4[b]	8	100	100 - 100	2	8	100	100 - 100	2
A/B/T	10[c]	20	100	100 - 100	4	20	100	100 - 100	4

[a] Uncertainty in feed flow rates.
[b] Uncertainty in feed flow rates and tray efficiency.
[c] Uncertainty in feed flow rates, efficiency and BIP's.

For the binary distillation cases, the OPT procedure coupled with CHEMCAD requires fewer MS's to converge than the SMSD procedure coupled with CHEMCAD does. However the computing time used by the OPT procedure coupled with CHEMCAD is larger than that used by the SMSD procedure coupled with CHEMCAD. This is probably due to EXCEL computations being slower than the C++ computations and to time required by the link between EXCEL and CHEMCAD.

4.8. Safety factor analysis for a distillation column case study

Purification of methanol by distillation is a necessary step in the production of high purity methanol from the coal gasification process. High crude oil prices and demand have motivated the search for alternative energy sources and chemical feed stocks. In the 1970's the use of methanol as a motor fuel received attention due to its availability, relatively low cost and environmental benefits. However, today its largest use is as chemical feed stock. In 2008 approximately 35% was converted to formaldehyde, and from there into products as diverse as plastics, plywood, paints, explosives, and permanent press textiles. Most of the methanol in the U.S. is produced from natural gas. However, coal is considered as the biggest potential source for methanol in the U.S because in the U.S. coal resources are larger than remaining natural gas and oil resources (Energy Information Administration, 2009). Nevertheless process economics are of paramount importance to favor the construction of coal to methanol plants. Purification of methanol by distillation may represent not only a large portion of the capital investment for the production of methanol from coal, but also a large part of the operating costs because it consumes a large amount of the energy.

This section analyzes the effect of safety factors on a methanol purification distillation column. PDR computations are obtained with the OPT procedure coupled with CHEMCAD.

The first step for the analysis is to obtain a nominal design. Then uncertainty in component feed flow rates is assumed and described by independent normal distributions. The PDR is estimated varying individually safety factors in number of trays and reboiler heat duty to observe the effect on the PDR. Then the sensitivity of the PDR to the flow rates uncertainty description, BIP's and tray efficiency is analyzed by reevaluating the PDR varying the flow rates uncertainty description, BIP's and tray efficiency.

4.8.1. Nominal design

Table 4.20 lists the data used for computing a distillation column nominal design. Component feed flow rates were taken from a coal gasification process' block flow material balance. Tray efficiency was selected based on the mixture type. For the thermodynamic database, the UNIQUAQ BIP's available from the CHEMCAD database were used.

A nominal design was obtained using the CHEMCAD shortcut and SCDS distillation column modules. Table 4.21 lists a summary of the nominal design. Note that the computed distillate meets the product specifications listed in Table 4.20. The EtOH in distillate is the limiting specification and locates the nominal design on the constraint boundary (CB) between the success and failure regions. By adding safety factors, the CB is normally moved away from the nominal design increasing the PDR.

Table 4.20. Data for computing nominal distillation column design.

Feed		
Pressure	50 psia	
Temperature	80 ^{o}F	
Methanol (MeOH)	14387 lbmol/hr	
Ethanol (EtOH)	100 lbmol/hr	
Water (W)	100 lbmol/hr	
Column		
Tray efficiency	60%	
Distillate specifications		
Distillate capacity	438753 lb/hr	
MeOH purity	$\geq$ 99.85% w/w (dry basis)	
EtOH content	$\leq$ 50 ppmw	
W content	$\leq$ 0.1% w/w	
Thermodynamic database (CHEMCAD UNIQUAC BIP's)		
Pair	$\lambda_{ij} - \lambda_{ii}$ (cal/gmol)	$\lambda_{ji} - \lambda_{jj}$ (cal/gmol)
MeOH – EtOH	-181.286	247.378
MeOH – W	95.259	-10.377
EtOH – W	50.88	232.01

Table 4.21. Summary of nominal distillation column design.

Distillation column specifications	
Condenser type	Total
Top pressure	16 psia
Condenser pressure drop	5 psi
Column pressure drop	5 psi
Stages	100
Feed stage	70
Tray efficiency	60%
Distillate mass flow rate	438752 lb/hr
EtOH bottoms mass flow rate	4585 lb/hr
Model output	
Methanol purity in distillate	99.995% w/w (dry basis)
Ethanol content in distillate	50 ppmw
Water content in distillate	7.4 E-7 % w/w
Reboiler duty	596,533,760 Btu/hr

4.8.2. Safety factor analysis

The effect on the PDR by the use of safety factors was studied. Safety factors in number of stages and reboiler heat duty were added separately.

To observe the PDR's sensitivity to the uncertainty's statistical description, the PDR was evaluated separately using three different standard deviations. The statistical descriptions used for the computations are listed in Table 4.22.

Table 4.22. Component feed flow rates' uncertainty described by normal distribution N(μ, σ^2).

Component	μ (lbmol/hr)	σ (lbmol/hr) S	σ_L (lbmol/hr) SL	σ_G (lbmol/hr) SG
MeOH	14387	1000	500	1500
EtOH	100	10	5	15
W	100	10	5	15

4.8.2.1 Effect on PDR by safety factor in number of stages

The PDR was estimated when adding 10, 20 and 30 stages above the feed stage. The number of stages and feed stage were modified in the CHEMCAD job project. The EXCEL file for the PDR estimation must be closed so the CHEMCAD job can be updated. The MC sets were updated using the statistical description group in turn from the groups listed in Table 4.22. Table 4.23 lists the common input data for the EXCEL file. The CHEMCAD BIP's used for computing the nominal design were also used here.

The estimated PDR's are presented in Figure 4.28. The graph shows that PDR increases as the number of stages increases. Also in this graph is observed that the increment in number of stages has a greater effect when the uncertainty in the component feed flow rates is low, i.e. smaller standard deviation, SL. Out of the nine designs only one design has an acceptable PDR. The distillation column with 130 stages and low uncertainty in component feed flow rates has a 94% PDR.

Table 4.23. Input data in EXCEL spreadsheet.

Seccion 1.	
Feed stream number	1
Distillate stream number	2
Bottoms stream number	3
Equipment ID	1
Feed option	2
Types of uncertainty	Component feed flow rates
Seccion 2.	
Feed temperature	80 ^{o}F
Feed pressure	50 psia
Nominal MeOH feed flow rate	14387 lbmol/hr
Nominal EtOH feed flow rate	100 lbmol/hr
Nominal W feed flow rate	100 lbmol/hr
Seccion 3.	
Nominal condenser specification	438753 lb/hr distillate
Nominal reboiler specification	4585 lb/hr EtOH in bottom product
Seccion 4.	
Condenser control variable	95% MeOH recovery in distillate
Reboiler control variable	596,533,760 Btu/hr
Seccion 5.	
Distillate constraint specification	$\geq$ 99.85% w/w MeOH (dry basis)
Distillate constraint specification	$\leq$ 50 ppmw EtOH
Seccion 6.	
Maximum step in linear search	3 σ
MC sets	10000

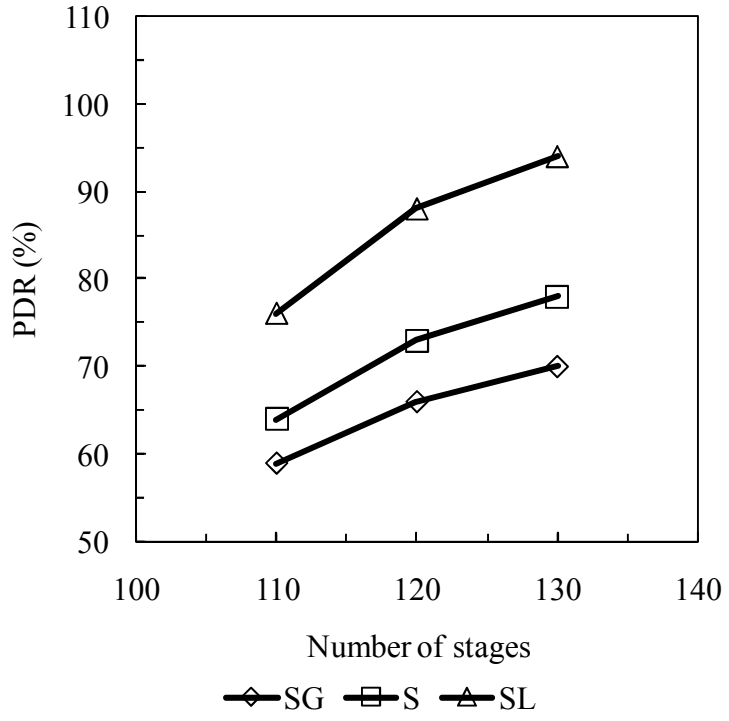


Figure 4.28. Effect on the PDR by adding safety factor to the number of stages and sensitivity to the change in component feed flow rate uncertainty.

4.8.2.2 Effect on PDR by safety factor in reboiler heat duty

The PDR was evaluated for designs with safety factor in reboiler duty varying from 4% to 20% of the reboiler duty computed with the nominal design, Table 4.21. The number of stages and feed stage were those computed for the nominal design, 100 and 70 respectively. With exception of the reboiler heat duty, the other input data in the EXCEL file are the same as those listed in Table 4.23. Also for the PDR computations of this section the CHEMCAD BIP's were used. The MC sets were updated using the statistical description group in turn from the groups listed in Table 4.22.

The estimated PDR's are shown in Figure 4.29. The PDR increases as the safety factor in reboiler duty increases. All the designs with low uncertainty, SL, have acceptable PDR's. However note that for low uncertainty more than 10% of safety factor is unnecessary. When the uncertainty is described by group S or SG a minimum safety factor in reboiler heat duty is required to obtain a PDR above 90%. When the uncertainty is S, a minimum safety factor of 8% in reboiler duty is required. When the uncertainty is SG, a minimum safety factor of 12% in reboiler duty is required. From comparing Figures 4.28 and 4.29, safety factors in reboiler heat duty have greater effect on the PDR than safety factors in number of trays.

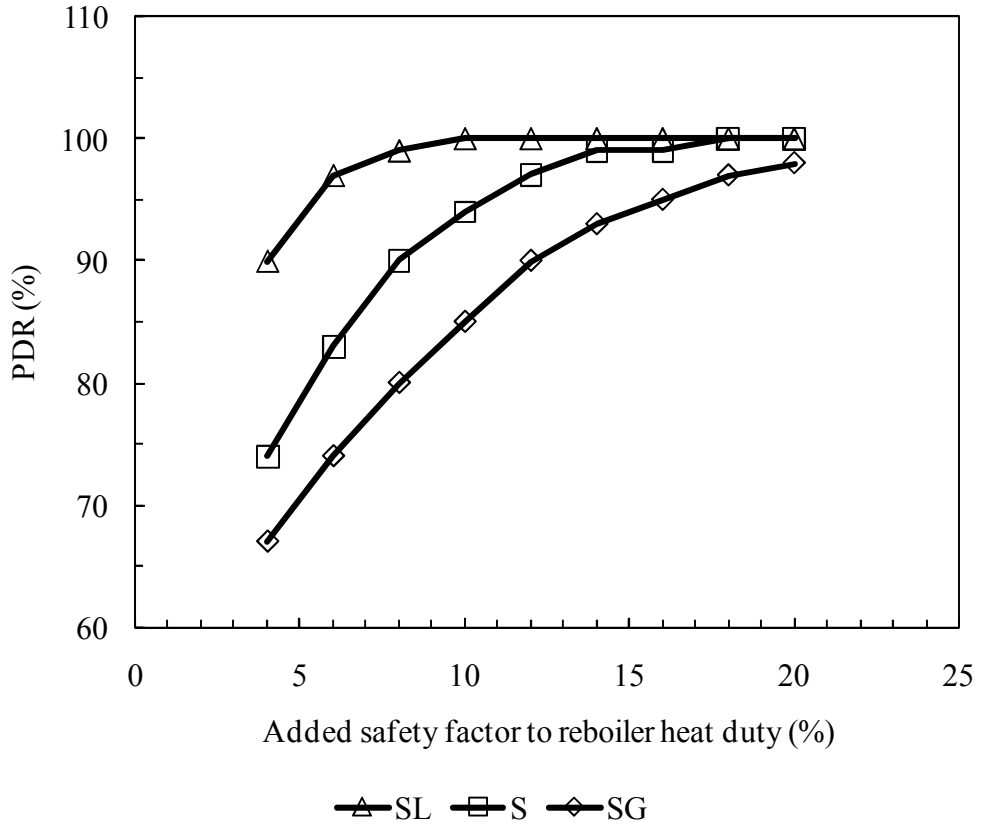


Figure 4.29. Effect in the PDR by adding safety factor to reboiler duty and sensitivity to the change in component feed flow rate uncertainty.

4.8.2.3 PDR's sensitivity to BIP's

The analysis presented in Sections 4.8.2.1 and 4.8.2.2 ignored the uncertainty in BIP"s. However, it is important to know the effect in the PDR by the BIP"s uncertainty and how the uncertainty in BIP's may be compensated by the use of safety factors.

The uncertainty in the CHEMCAD BIP's is unknown, so there are not statistical descriptions that could be included for evaluating the PDR's. Instead, it is assumed that the actual thermodynamic behavior of the mixture is described by a different group of BIP's. Therefore the nominal design is developed using the CHEMCAD BIP's,G1; but the MS's required by the PDR estimating procedure use the group of BIP's that describe the actual behavior of the mixture, G2. The same safety factors used in Sections 4.8.2.1 and 4.8.2.2 are used to evaluate the PDR's and the results are compared with the ones obtained in those sections. The common input data for the EXCEL file are the same listed in Table 4.23.

The group of BIP's G2 used for describing the actual behavior of the mixture is listed in Table 4.24. Two pairs of BIP's are the same provided by CHEMCAD. However, the pair for the EtOH and MeOH was replaced by a different pair. This pair was obtained by regression of an experimental data set taken from Gmehling (1977). The CHEMCAD BIP regression tool was used. The experimental data set is listed in Appendix B.

Table 4.24. BIP"s used for sensitivity analysis, G2.

Pair	$\lambda_{ij} - \lambda_{ii}$ (cal/gmol)	$\lambda_{ji} - \lambda_{jj}$ (cal/gmol)
MeOH – EtOH (regressed)	146.9225	-116.9267
MeOH – W (CHEMCAD)	95.259	-10.377
EtOH – W (CHEMCAD)	50.88	232.01

Figures 4.30 and 4.31 show the PDR's obtained using the new group of BIP's, G2, and the results presented in Sections 4.8.2.1 and 4.8.2.2. Both figures show significant

changes in the PDR's. In both figures more designs have acceptable PDR's when using the BIP's from group G2 than when using the BIP's from G1. This is because when using group G1 the number of stages or reboiler heat duty requirements are larger to meet product specifications than when using group G2. From this example it is conclude that ignoring the uncertainty in BIP's may result in equipment over-sizing and incurring in unnecessary costs.

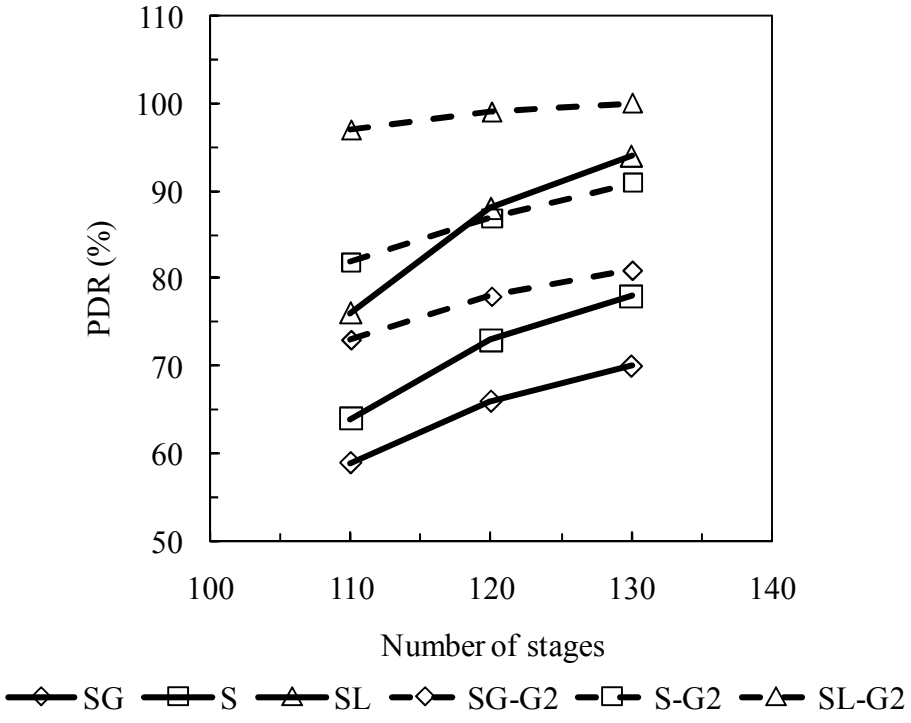


Figure 4.30. Effect in the PDR by adding safety factor to the number of stages and sensitivity to the change in component feed flow rate uncertainty and BIP's.

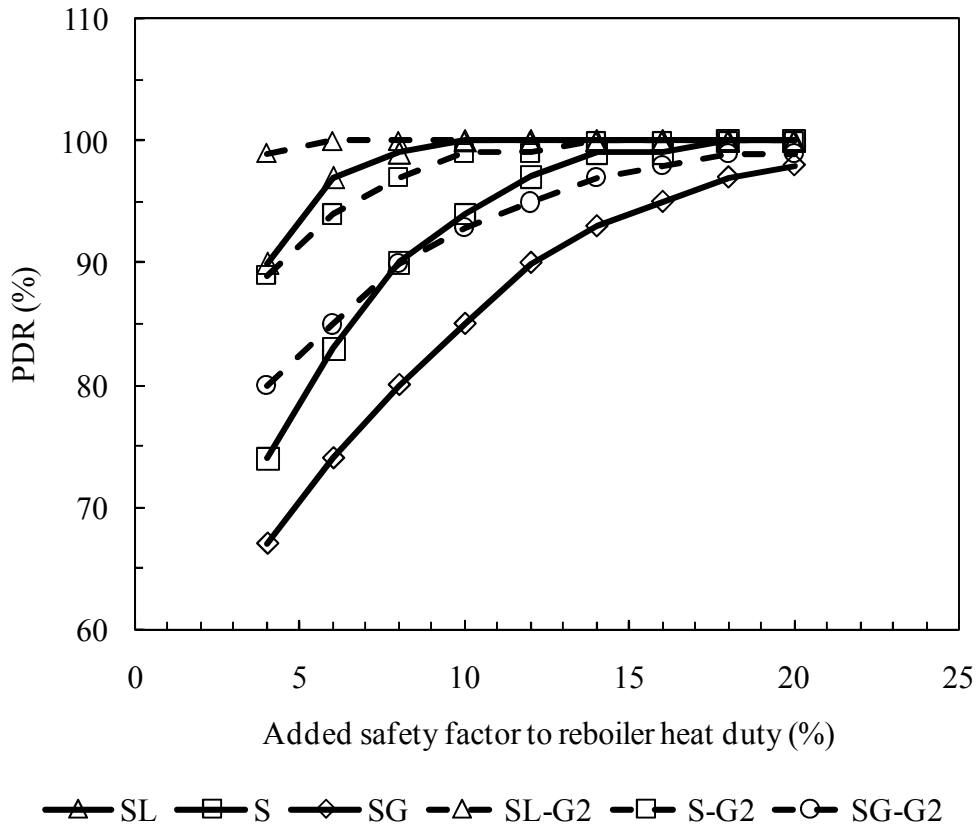


Figure 4.31. Effect in the PDR by adding safety factor to reboiler duty and sensitivity to the change in component feed flow rate uncertainty and BIP's.

4.8.2.4. PDR's sensibility to tray efficiency

The analysis of this section is similar to the analysis of the previous section. The analysis presented in Sections 4.8.2.1 and 4.8.2.2 ignored the uncertainty in tray efficiency. So the goal here is to observe the effect on the PDR when the distillation column's tray efficiency during normal operation is different of that one used for developing the nominal design and selecting safety factors. Also for this section PDR of the designs described in Sections 4.8.2.1 and 4.8.2.2 were used for re-estimating the PDR, but using different tray efficiency. In this case a tray efficiency of 55% is used.

Figures 4.32 and 4.33 present the results of this section and those from Sections 4.8.2.1 and 4.8.3.2. For all designs the PDR decreases. Only when using safety factors in reboiler heat duty some of the PDR's are of 90% or higher. The use of this type of results may help to avoid under-sizing equipment.

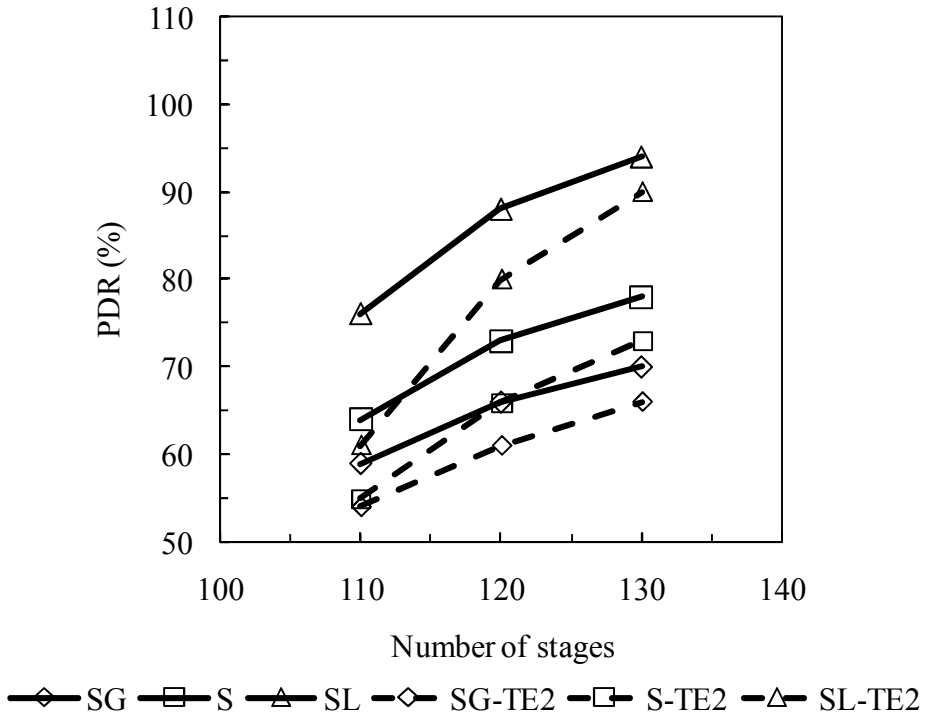


Figure 4.32. Effect in the PDR by adding safety factor to the number of stages and sensitivity to the change in component feed flow rate uncertainty and tray efficiency.

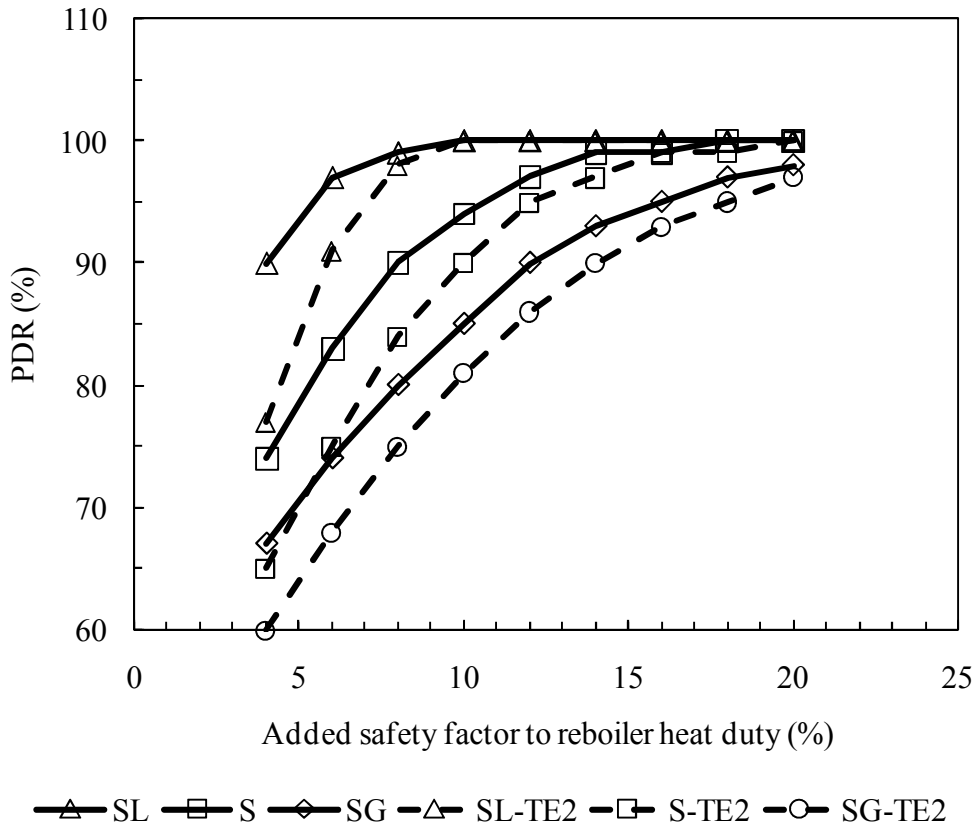


Figure 4.33. Effect in the PDR by adding safety factor to reboiler duty and sensitivity to the change in component feed flow rate uncertainty and tray efficiency.

4.9. Conclusions and recommendations

Two efficient procedures to estimate PDR have been coupled with a widely available commercial process simulator. Also the use of the PDR estimating results for safety factor selection was demonstrated with a case study. This makes available to practicing engineers a computationally efficient tool to estimate process design reliability and better evaluate the capital required to add flexibility and capacity to cope with uncertainties.

The computational efficiency of the SMSD and OPT procedures coupled with CHEMCAD has been tested with distillation column designs. The initial accuracy of the

tangential OPT PDR estimates has been improved by coupling the OPT procedure with CHEMCAD. Initial tangential OPT PDR estimates are within 3.5% error with respect to CMCI PDR estimates. For designs with two uncertain parameters the OPT procedure required less BP's and MS's than the SMSD procedure did. However the coupling with the EXCEL integration method makes the OPT procedure slower than the SMSD procedure is. Nonetheless the SMSD and OPT procedures require two to three orders of magnitude less MS's and computing time than the CMCI procedure does.

Extending the use of the SMSD procedure coupled with CHEMCAD for estimating the PDR of designs with more than two uncertain parameters may be possible by improving the method for constructing the CBA. This may be done by increasing the number of initial BP's and developing an efficient method for connecting them.

To improve the OPT procedure's computational efficiency it is recommended that future work focus on: 1) the improvement of the pessimistic CBA approach to reduce the uncertainty in the PDR estimates and faster the procedure's convergence; 2) the development of an efficient procedure to evaluate the convergence of the procedure; and 3) the improvement of the line-search procedure to reduce the number of MS's required per BP.

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Chapter 5
Conclusions and Recommendations

5.1. Conclusions

The goals of developing a computationally efficient method to estimate design reliability and coupling the method with a commercially distributed process simulator were met. The method can now be used by the process design community.

The OPT procedure developed by MacDonald (1993) was updated to run in the Microsoft Windows environment. For the distillation case studies considered in this work, the OPT procedure was two to three orders of magnitude faster than CMCI. The tangential approximation provided accurate PDR estimates, usually within 1.5% deviation with respect the CMCI PDR estimate, for a reasonable number of MS's. However as the number of uncertain parameters increases the advantage of the OPT procedure over CMCI is reduced.

A modified version of the OPT procedure, the SMSD procedure, was developed and tested. Tests with geometrical and distillation designs show that the ability of the SMSD procedure strongly depends on the CB's shape and number of parameters. For some of the considered designs, the SMSD procedure was able to compute more accurate PDR estimates with fewer MS's than the OPT procedure did, even when sometimes the SMSD procedure required more BP's. For designs with more than two uncertain parameters the SMSD procedure was not able to approximate the design's CB accurately.

The OPT and SMSD procedures were coupled with a widely available commercial process simulator. This coupling makes PDR estimation available to practicing engineers.

The computational efficiency of the SMSD and OPT procedures coupled with CHEMCAD was tested with distillation column designs. The initial accuracy of the tangential OPT PDR estimates was improved by coupling it with CHEMCAD. Initial tangential OPT PDR estimates are within 3.5% error with respect to CMCI PDR estimates. Final tangential OPT PDR estimates are within 1.3% error with respect to CMCI PDR estimates. With exception of the M/I design with five uncertain parameters the OPT procedure meets the convergence criteria and uses a reasonable number of MS's for it. For the designs with two uncertain parameters the OPT procedure required less BP's and MS's than the SMSD procedure did. However the coupling with the EXCEL integration method makes the OPT procedure to be slower than the SMSD procedure coupled with CHEMCAD using the UAM method is. The SMSD and OPT procedures are two to three orders of magnitude computationally more efficient than the CMCI procedure.

5.2. Recommendations

Extending the use of the SMSD procedure coupled with CHEMCAD for estimating the PDR of designs with more than two uncertain parameters may be possible by improving the method for constructing the CBA. This may be done by increasing the number of initial BP's as dimension increases and developing a new method for connecting them.

For the case studies considered in this work the initial tangential OPT PDR estimates were sufficiently accurate. However it may not always be the case. The addition of BP's to improve or verify the estimate's accuracy reduces considerably the

procedure's computational efficiency. A computationally efficient method for determining the convergence of the procedure needs to be developed.

Improvement of the line-search procedure for searching BP's is recommended to improve the SMSD or the OPT procedures' computational efficiency.

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APPENDIX A
Description of computer programs

A.1. OPT FORTRAN programs

A.1.1. For distillation column case studies

The simulator developed by McDonald (1993) was adapted to be compiled with Compaq Visual FORTRAN. The simulator that was available for starting this work missed the file that contained the code for: 1) executing sequentially the computations of the first iteration of the procedure; and 2) linking the main OPT procedure's computations with the line-search computations. Therefore the necessary code was written and a new form to link the main computations with the line-search computations was developed.

The code for the new OPT program is built into a workspace named DREWorkIMSL and composed by two projects: DREWorkIMSL and DISTRUN. Figure A.1 presents a screen shot of the Compaq Visual environment showing the DREWorkIMSL workspace. The DREWorkIMSL project is the main project and computes the main calculations of the OPT procedure. The DISTRUN project is defined as a dynamic link library (DLL) and is called by the DREWorkIMSL project to execute the line-search computations.

The DREWorkIMSL project is made up of 40 files. Ten of these files are external dependencies, i.e. they contain definition of variables and common data blocks. The rest contain the main program, subroutines and functions. Table A.1 lists the files that contain the main program, subroutines and functions, including a short description of those subroutines and functions. Table A.2 contains the list of the external dependencies.

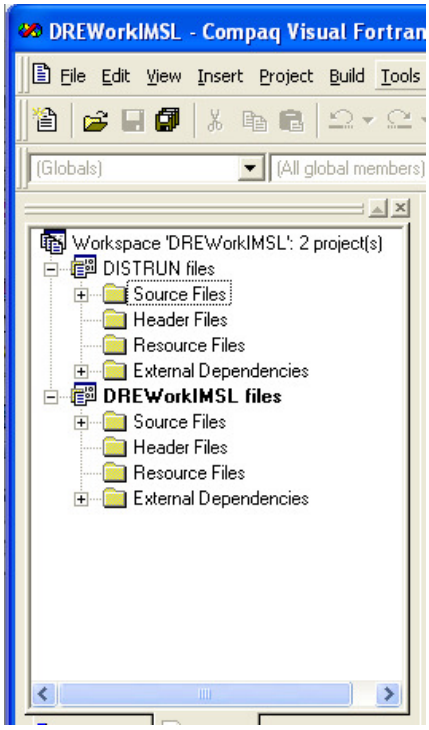

Figure A.1. Screen shot that shows the DREWorkIMSL workspace.

The DISTRUN project contains the code for the computations of the line-search procedure, including the distillation column simulation. This project is made up of 64 files. Eighteen of these files are external dependencies used also for defining variables and common data blocks. The rest of the files contain subroutines and functions. The list of subroutines and functions with a short description are presented in Table A.3. Table A.4 contains the list of external dependencies.

To run the program outside the Compaq Visual environment eight files are necessary. These files need to be in the same directory. The files are: the executable file (DREWorkIMSL.exe), the DLL file (DISTRUN.dll) and six data files from where the program obtains necessary information for the computations. A screen shot of an example case study directory is shown in Figure A.2. The list of the data files with a brief description is given in Table A.5.

Table A.1. Subroutines and functions of the DREWorkIMSL project.

File	Subroutine or Function	Description
DREWorkIMSL.f90	desuncert	Main program for running the OPT procedure.
	datafile	Reads information from file FileOPTData.txt.
	setseeds	Initializes random number seeds.
addrad.f90	addrad	Writes search radial directions into file !RunRadList.
bndry.f90	bndry	Subroutine to compute the CBA planes. It is also used to save information in BndryInfo file
inconn.f90	incon2	Checks if a MC set is within the connecting-plane CBA of a NNG.
inconn.f90	inconn	Control subroutine to check if a MC set is within the connecting-plane boundary of a NNG.
intan.f90	intan	Checks if a MC set is within the tangent-plane CBA of a NNG.
intdsu.f90	intdsu	Initializes CBA variables.
matmul.f90	matmul	Multiplies two matrices.
matslv.f90	matslv	Computes matrix inversion with maximum pivoting.
mcgen.f90	mcgen	Generates MC set. Uses IMSL libraries to compute random normal or uniform numbers.
mcintg.f90	mcintg	Performs MCI.
neigha.f90	neigha	Adds a new BP to the NNG matrix.
neighb.f90	neighb	Calculates the hyper-planes that define the space of each NNG.
neighd.f90	neighd	Enumerates the initial NNG's and later it is used for determining in which quadrant a new point is in.
neighi.f90	neighi	Initializes the NNG matrix.
neighp.f90	neighp	Computes connecting-planes of NNG's.
neighs.f90	neighs	Checks if each NNG has the same common active constraint.
neight.f90	neight	Determines the type of curvature of NNG's.
neighw.f90	inchck	Checks if a MC set falls in the space of a NNG.
	neighw	Controls the search of the NNG in which a MC set falls in.
nxtrad.f90	nxtrad	Computes the next radial direction to search for BP.
rand.f90	randmod	Generates a random number. It uses Compaq FORTRAN 90 library function RANDOM.
randnm.f90	randnm	Generates a uniform random number and transforms it to a number with normal distribution.
redinitbp.f90	redinitbp	Performs the initial boundary approximation and call for the MC integration.

Table A.1. (Continuation.)

File	Subroutine or function	Description
rednew.f90	rednew	Reads the new BP that is stored in the temporary file !NewBndryPts and saves it to the permanent file !BndryPts. Updates the NNG's matrix.
redprj.f90	redprj	Reads distillation column information, including nominal parameter values, from file !Ctrl.
redpts.f90	redpts	Reads the !BndryPts file.
sdvdst.f90	sdvdst	Calculates multiplier used to obtain the radial vector for the next search.
statdat.f90	statdat	Reads the parameter statistical descriptions from file control2b.txt.
strtup.f90	strtup	Calls subroutines redprj and statdat to read data files.
tanclc.f90	tanclc	Checks if a MC set is inside or outside the tangential plane approximations.
zero.f90	zero	Subroutine to zero all elements of an array.

Table A.2. Description of external dependency files of the DREWorkIMSL project.

File	Description
ctrlcom.fi	Declares common blocks for project name variables.
ctrldec.fi	Declares project name variables.
desunccom.fi	Declares common blocks for design reliability variables.
desuncdec.fi	Declares variables for the design reliability calculations
dimencom.fi	Declares common blocks for maximum dimensions
distcom.fi	Declares common blocks for distillation column variables
distdec.fi	Declares variables for distillation column
maxdimen.fi	Declares maximum dimensions of vectors (streams, stages, etc)
statcom.fi	Declares common blocks for statistical description of the uncertain parameters.
statdec.fi	Declares variables for the statistical description of the uncertain parameters.

Copy of initial files required for each of the case studies presented in Chapter 2 and Chapter 3 is provided in the attached CD under the directory OPTCaseStudies. During the execution of the procedure the program creates the seven files listed in Table A.6.

To edit the OPT program in a different computer is necessary to have a copy the whole workspace, i.e. the directory DREWorkingIMSL. Copy of this workspace is included in the attached CD under the directory OPTWorkspace.

Table A.3. Subroutines and functions of the DISTRUN project.

File	Subroutine or function	Description
dstrunrad.f90	distrunrad	Main subroutine of the distillation simulator.
	edpeqp	Edits equipment data (distillation column).
	oldprj	Prompts the user for an old project name and reads it into memory
acalc.f90	acalc	Calculates the A Jacobian matrix for the *i*-th stage.
addstp.f90	addstp	Adds the Newton step to the unknown variables.
	dmpstp	Dampens the steps for the Newton iteration by simply multiplying all the steps by the specified damping factor.
	maxstp	Limits the maximum allowable step values for the Newton iteration.
bcalc.f90	bcalc	Calculates the B Jacobian matrix for *i*-th stage.
blkinv.f90	blkinv	Calculates the next Newton step in the unknown variables.
botclc.f90	botclc	Calculates the extra independent specification for the bottom stage.
bubp.f90	bubp	Finds saturated pressure at the bubble point temperature.
bubt.f90	bubt	Finds saturated temperature at bubble point.
ccalc.f90	ccalc	Calculates the C Jacobian matrix for *i*-th stage.
chkcnv.f90	chkcnv	Calculates the function residuals and check for convergence
dbread.f90	dbread	Read the physical property database files
dewp.f90	dewp	Finds the saturated pressure at the dew point temperature.
	dpeqns	Calculate the functions to be converged for the dew point pressure calculation.
	dpjac	Calculates the analytical values for the Jacobian for the dew point calculation.
dewt.f90	dewt	Finds saturated temperature at dew point
	dteqns	Calculates residual functions for the dew point temperature calculation.
	dpjac	Calculates analytical values for the Jacobian approximation for the dew point calculation.
dstini.f90	dstini	Initializes the distillation variables, most of them to a zero value and some of them to other default values.
dstout.f90	dstout	Subroutine called when the distillation has converged to save the product streams back into the stream array.
dstrad.f90	dstrad	Controls line-search procedure computations.
	gcalc	Calculates the residual inequality constraint.
	thtset	Puts the current value of the distillation parameters into memory.

Table A.3. (Continuation.)

File	Subroutine or Function	Description
dstred.f90	dstred	Reads the distillation input file which contains specifications and initial variable estimates.
dstrun.f90	dstrn2	Computes the Napthali-Sandholm iteration. It sends the convergence criteria results to dstrun.
	dstrun	Controls the Napthali-Sandholm method..
dtbase.f90	dtbase	Controls calculations of k-values and/or enthalpy.
energy.f90	energy	Calculates energy balance residual for a given stage.
enthkv.f90	enthkv	Calculates the K-value and enthalpy for a given stage.
enthlp.f90	enthlp	Calculates the molal enthalpies for the liquid and vapor streams. Also calculates pure component enthalpies for use with partial derivative approximations.
htduty.f90	htduty	Calculates the condenser and reboiler heat duty once the convergence criteria have been met, or when called by the printing subroutine to print iteration results for debugging purposes.
intsim.f90	intsim	Initializes all the variables.
jacob.f90	jacob	Calculates the Jacobian for the Napthali-Sandholm method.
	niljac	Zeros the Jacobian matrices.
kval.f90	cubic	Calculates the analytical roots of a cubic equation.
	kval	Rigorously calculates k-values.
ldens.f90	ldens	Calculates molar volumes of pure saturated liquid components.
liq2ph.f90	lilik	Calculates the liquid-liquid equilibrium k-values.
	liq2ph	Calculates the liquid phase activity coefficients.
liqgam.f90	liqgam	Rigorously calculate the liquid activity coefficients.
lvnorm.f90	lvnorm	Calculates total vapor and liquid flow rates
mass.f90	mass	Calculates the mass balance equations for the given stage.
matmul.f90	matmul	Multiplies matrices.
matslv.f90	matslv	Matrix inversion program with maximum pivoting.
mesh.f90	mesh	Calculates the MESH equations for all stages.
molwt.f90	molwt	Calculates the molecular weight of a given stream.
phase.f90	phase	Calculates the E equations for the given stage.
prtitr.f90	prtitr	Prints the MESH function residuals for each stage for iteration.
prtjac.f90	prtjac	Prints the Jacobian matrices to the iteration file if it is required.
prtstp.f90	prtstp	Prints Newton steps to the iteration file.
psat.f90	psat	Calculates pure component vapor pressures.

Table A.3. (Continuation.)

File	Subroutine or Function	Description
sfileman.f90	filesub	Solves the frequent problem of having to delete file itr; decides the way a file is going to be open.
stepp.f90	stepp	Steps unknown variables (x) by the residual value.
strprp.f90	strprp	Calculates physical properties of stream array.
strqal.f90	strqal	Calculates quality of a stream given a variety of conditions.
topclc.f90	topclc	Calculates the extra independent specification for the top stage.
zero.f90	zero	Subroutine to zero all elements of an array.

Table A.4. Description of external dependency files of the DISTRUN project.

File	Description
DBaseCom.fi	Declares common blocks of physical properties.
DBaseDec.fi	Declares physical properties variables.
DCtrlCom.fi	Declares common blocks for project names variables.
DCtrlDec.fi	Declares project control name variables.
DDimenCom.fi	Declares common blocks of dimension size variables/parameters.
DDistCom.fi	Declares common blocks of dimension tower variable arrays.
DDistDec.fi	Declares dimension tower variable arrays.
DMaxDimen.fi	Declares maximum dimensions.
FlshCom.fi	Declares common blocks of flash specification/control array.
FlshDec.fi	Declares flash specification/control array.
IterCom.fi	Declares common blocks of iteration variables.
IterDec.fi	Declares iteration variables.
MESHCom.fi	Declares common blocks of MESH equations.
MESHDec.fi	Declares MESH equations.
PartCom.fi	Declares common blocks of partial derivatives.
PartDec.fi	Declares partial derivatives.
SimCom.fi	Declares common blocks of stream array.
SimDec.fi	Declares stream array.

Table A.5. Description of input data files required by the DREWorkIMSL workspace.

File	Information
!control	Name of file from where to read component property constants. Distillation case information.
control2b.txt	Statistical description of parameters.
!ctrl	Distillation case specifications.
database.txt	Constants to compute component properties.
dist	Distillation case specifications and initial guess values for Naphtali- Sandholm method.
FileOPTData.txt	Number of MC sets, step size in line-search procedure and options for convergence criteria.

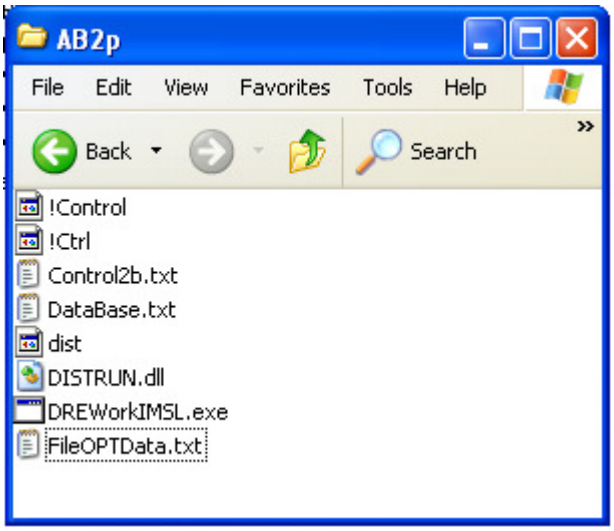

Figure A.2. Screen shot of an example of case study directory.

Table A.6. Data files created by the DREWorkIMSL.exe program.

File	Information
BndryInfo	Initial NNG's borders and connecting and tangential planes.
!bndrypts	BP's, active constraint, gradients and MS's used to find each BP.
MCpoints1stIter.txt	Location of each MC set in the initial NNG's.
MCpoints1stFinal.txt	MCI statistics for the final CBA's.
!NewBndryPts	Intermediate file with BP information.
!RunRadList	Radial direction(s).
ZSDRE.txt	Summary of MCI statistics.

A.1.2. For geometrical case studies

The program for estimating PDR of geometrical designs is built into a workspace named DREIMSLGeo and composed by the project: DREIMSLGeo. The workspace does

not require a DLL for the line-search procedure because the geometrical designs are modeled by simple equations in terms of the uncertain parameters. The code from the DREWorkIMSL project was used as the base for developing the DREIMSLGeo project. The DREIMSLGeo project is formed by 34 files. 24 of these files contain subroutines and/or functions and the rest of them are external dependencies. Table A.7 presents the list of files containing subroutines or functions. Table A.8 describes the content of the file dreimslgeo.f90. The description of the other files is omitted since is the same than that given in Table A.1. Table A.9 presents the list of external dependencies.

Table A.7. DREIMSLGeo project's files with subroutines and/or functions.

addrad.f90	matmul.f90	neighd.f90	nextrad.f90
bndry.f90	matslv.f90	neighi.f90	redinibp.f90
dreimslgeo.f90	mcgen.f90	neighp.f90	rednew.f90
inconn.f90	mcintg.f90	neighs.f90	statdat.f990
intan.f90	neigha.f90	neight.f90	tanclc.f90
intdsu.f90	neighb.f90	neighw.f90	zero.f90

Table A.8. Subroutines or functions in file dreimslgeo.f90.

Subroutine or function	Description
desuncert	Main subroutine to control sequential computations
readchangedata	Reads data from file OPTGeoData.txt
linesearch	Computes line-search procedure
ggcalc	Computes constraint equations
setseeds	Initialize random number seeds
newresfile	Saves MCI results

Table A.9. DREIMSLGeo project's external dependencies.

ctrlcom.fi	desuncdec.fi	geodec.fi	statdec.fi
ctrldec.fi	dimencom.fi	maxdimen.fi	
desunccom.fi	geocom.fi	statcom.fi	

To run the program outside the Compaq Visual environment it is required to have in the same directory the executable file (DREIMSLGeo.exe) and the file OPTGeoData.txt. The latter file contains: the number of MC sets to use in the MCI, the maximum number of BP's to use for the CBA, the initial step size to use for the line-search of the axial

BP's, the initial step size to used for the line-search of additional BP's and the convergence criteria for the line-search procedure. The program may generate the files listed in Table A.17. A copy of the DREIMSLGeo workspace is provided in the attached CD under the directory OPTGeoWorkspace.

A.2. CMCI FORTRAN program

A.2.1. For geometrical case studies

The program for estimating PDR of geometrical cases by CMCI is built into the Visual FORTRAN workspace DRCMCGeoIMSL. This workspace contains only one project that has the same name as the workspace. This project is made up of fourteen files. Four of these files contain the code for the computations of the procedure and the other ten files are external dependencies. Tables A.10 and A.11 have the list of those files with a brief description of their content.

Table A.10. Subroutines and functions of the DRCMCGeoIMSL project.

File	Subroutine or Function	Description
DRCMCGeo IMSL.f90	DRCMCGeoIMSL	Main program for CMCI for geometrical cases.
	newdata	Sets values to variables.
	ggcalc	Evaluates the residual inequality constraints.
	setseeds	Initializes random number seeds.
intdsu.f90	intdsu	Initializes CBA variables.
mcgen.f90	mcgen	Generates MC set. Uses IMSL libraries to compute random normal or uniform numbers.
statdat.f90	statdat	Reads the parameter statistical descriptions.

To run the program outside the Compaq Visual FORTRAN environment it is necessary to have only the file DRCMCGeoIMSL.exe. The program generates two files with results: DRCMCGeo.txt and DRCMCGeoDisCon.txt. A copy of the DRCMCGeoIMSL workspace can be found in the attached CD in the directory CMCIGeoWorkspace.

A.2.2. For distillation case studies

The program for estimating PDR of distillation designs by CMCI is built into the Visual FORTRAN workspace DRCMCII. This workspace contains two projects, one with the same name as the workspace and one named DISTCOL. The DRMCII project is made up of nineteen files from which nine contain the code of the computations and the other ten are external dependencies. Table A.12 lists the nine files with a brief description of their content. The external dependencies are the same as those listed and described in Table A.2.

Table A.11. Description of external dependency files of the DRCMCGeoIMSL project.

File	Description
ctrlcom.fi	Declares common blocks for project name variables.
ctrldec.fi	Declares project name variables.
desunccom.fi	Declares common blocks for design reliability variables.
desuncdec.fi	Declares variables for the design reliability calculations
dimencom.fi	Declares common blocks for maximum dimensions
geocom.fi	Declares common blocks for geometrical case variables.
geodec.fi	Declares variables for geometrical case.
maxdimen.fi	Declares maximum dimensions of vectors.
statcom.fi	Declares common blocks for the uncertain parameter statistical descriptions.
statdec.fi	Declares variables for the uncertain parameter statistical descriptions.

The DISCOL project is defined as a DLL and is made up of 64 files. Eighteen of those files are the same as the external dependencies listed and described in Table A.4. The other forty six files contain the code for the distillation column simulation for each MC set of uncertain parameters. Forty five of those files have the same name as those files listed in Table A.3. Instead of having a file named dstrunrad.f90 the DISCOL project has a file named discol.f90. The discol.f90 file contains code for initializing variables for running the distillation model simulations. With exception of the file dstrad.f90 the description of files given Table A.3 is the same for the files contained in

the DISCOL project. The description of the subroutines in the file dstrad.f90 is given in Table A.13.

Table A.12. Subroutines and functions of the DRCMCII project.

File	Subroutine or Function	Description
DRCMCII.f90	DRCMC	Main program for CMCI of distillation case studies.
	filecheck	Checks the existence of file. If the file does exist then it overwrites on it, otherwise creates a new file with the specified name.
	newdatafile	Reads data from file FilCasData.txt.
intdsu.f90	intdsu	Initializes CBA variables.
mcgen.f90	mcgen	Generates MC set. Uses IMSL libraries to compute random normal or uniform numbers.
rand.f90	randmod	Generates a random number. It uses Compaq Fortran90 library function RANDOM.
randnm.f90	randnm	Generates a uniform random number and transforms it to a number with normal distribution.
redprj.f90	redprj	Reads distillation column information, including nominal parameter values, from file !Ctrl.
statdat.f90	statdat	Reads the parameter statistical descriptions.
strtup.f90	strtup	Calls subroutines redprj and statdat to read data files.
zero.f90	zero	Subroutine to zero all elements of an array.

Table A.13. Subroutines in file dstrad.f90 of the DISTCOL project.

Subroutine or Function	File	Description
dstrad.f90	dstrad	Controls distillation model simulation.
	gcalc	Calculates the residual inequality constraints.
	thtset	Puts the current value of the distillation parameters into memory.

The DRCMCII workspace requires six input data files which are listed in Table A.14. To run the program outside the Compaq Visual environment it is required to have in the same directory the executable file (DRCMC.exe), the DLL (DISTCOL.dll) and the six data files. The program saves the results in the file CMCDRERes.txt . A copy of the DRCMCII workspace is included in the attached CD under the directory CMCIWorkspace.

Table A.14. Description of input data files required by the DRCMCII workspace.

File	Information
!control	Name of file from where to read component property constants. Distillation case information.
control2b.txt	Statistical description of parameters.
!ctrl	Distillation case specifications.
database.txt	Constants to compute component properties.
dist	Distillation case specifications and initial guess values for Naphtali- Sandholm method.
FilCasData.txt	Data related to parameter uncertainty description and MCI.

A.3. SMSD FORTRAN programs

A.3.1. For geometrical case studies

The program for estimating PDR of geometrical designs is contained in the workspace named DREMODGeoIMSL. This workspace contains only one project that has the same name as the workspace. This project is made up of thirty five files. Twenty five of these files contain the code for the computations of the procedure and the other ten files are external dependencies. The external dependencies are the same listed in Table A.11. Table A.15 lists the files containing the code. The workspace was developed with the initial idea of having the option to run either the OPT or the SMSD procedure. Because of that the files containing subroutines and functions used by the OPT procedure with the tangent plane approximation are included in Table A.15. Later it was decided that it was easier to keep a program for each procedure option. However the unnecessary files for the SMSD procedure were not removed. The description of the files is the same as that given in Table A.1. Table A.16 describes the content of the DREMODGeoIMSL.f90 file.

To run the program outside the Compaq Visual FORTRAN environment it is necessary to have only the file DREMODGeoIMSL.exe. The program may generate the

five files listed in Table A.17. A copy of the DREMODGeoIMSL workspace can be found in the attached CD under the directory DREMODGeoWorkspace.

Table A.15. Files containing code for the DREMODGeoIMSL workspace.

addrad.f90	intdsu.f90	neigha.f90	rednew.f90
bndry.f90	matmul.f90	neighb.f90	statdat.f90
dremodgeoimsl.f90	matslv.f90	neighd.f90	strup.f90
inconn.f90	mcgen.f90	neighi.f90	tanclc.f90
intan.f90	mcintg.f90	neighp.f90	zero.f90

Table A.16. Description of content in file DREMODGeoIMSL.f90.

Subroutine or function	Description
desuncert	SMSD procedure's main program for geometrical designs.
filesub	Checks the existence of file. If the file does exist then it overwrites on it, otherwise creates a new file with the specified name.
ggcalc	Computes residual of constraint equations.
linesearch	Computes line-search procedure.
newdata	Sets program control values.
newresfile	Prepares files to save results.

Table A.17. Data files created by the DREMODGeoIMSL workspace's code.

File	Information
ZSDRE.txt	Summary of MCI statistics after each addition of BP's.
SummaryERM.txt	MCI and next search results after each addition of BP's.
SummaryERM2.txt	MCI results at initialization for each of the MC sets.
SummaryERM3.txt	Final MCI results of the CBA for each NNG.
SummaryERM4.txt	Computed statistical distances computed after each MCI.

A.3.2. For distillation case studies

The program for estimating PDR of distillation designs is contained in the workspace named DREMOD_IMSL_3. This workspace contains two projects: DREMOD_IMSL_3 and DISTRUN. The DISTRUN project is defined as a DLL and is made up of 64 files listed and described in Tables A.3 and Table A.4 with exception of the subroutine dstrad in file dstrad.f90. This subroutine's code corresponds to the line-search procedure. For the SMSD procedure it is not required to compute partial derivatives at each BP.

The DREMOD_IMSL_3 project is made up of forty files. Thirty of these files contain the code for the computations of the procedure and the other ten files are external dependencies. The external dependencies are the same listed in Table A.2. Table A.18 lists the files containing the code of the procedure. Table A.19 describes the content of the dremod_imsl3.f90 file. The content of the other twenty nine files is the same as that described in Table A.1.

Table A.18. Files containing code for the DREMODGeoIMSL workspace.

addrad.f90	mcgen.f90	neight.f90	redpts.f90
bndry.f90	mcintg.f90	neighw.f90	sdvdst.f90
dremod_imsl3.f90	neigha.f90	nexrad.f90	statdat.f90
inconn.f90	neighb.f90	rand.f90	strup.f90
intan.f90	neighd.f90	randnm.f90	tanclc.f90
intdsu.f90	neighi.f90	redinibp.f90	zero.f90
matmul.f90	neighp.f90	rednew.f90	
matslv.f90	neighs.f90	redprj.f90	

Table A.19. Description of file DREMODGeoIMSL.f90's content

Subroutine or function	Description
dremod_imsl3	SMSD procedure's main program for distillation designs.
newdatafile	Sets program control values.
newresfile	Prepares files to save results.
setseeds	Initializes seeds for random number generation.

To run the program outside the Compaq Visual FORTRAN environment it is necessary to have the files: DREMOD_IMSL_3.exe, DISTRUN.dll and the six data files listed in Table A.14. In addition to the information described to be contained in file FilCasData.txt, it also contains information related to initial step sizes in the line-search procedure and convergence criteria of SMSD procedure. The program may generate the six files listed in Table A.21. The results in some of those files were used to evaluate the procedure's performance, but may not always be necessary. A copy of the

DREMOD_IMSL_3 workspace can be found in the attached CD under the directory DREMODWorkspace.

Table A.20. Data files created by the DREMOD_IMSL_3.exe program.

File	Information
ZSDRE.txt	Summary of MCI statistics after each addition of BP's.
SumMCPointsRes.txt	Final MCI results for each MC set.
SummaryERM.txt	MCI and next search results after each addition of BP's.
SummaryERM2.txt	MCI results at initialization for each of the MC sets.
SummaryERM3.txt	Final MCI results of the CBA for each NNG.
SummaryERM4.txt	Computed statistical distances computed after each MCI.

A.4. OPT and CMCI programs in EXCEL/VBA

The code for the OPT and CMCI programs was written under the EXCEL Visual Basic Application editor environment. The two procedures share some of the subroutines and functions. The complete list of subroutines and functions and a brief description of them is given in Table A.21. Data for running the OPT and CMCI computations is taken from the EXCELsheets: DataResSum, BIPsStatDes and MCPoints. Cells with light gray background in the sheets DataResSum and BIPStatDes indicate that is information that needs to be provided by the user or taken from CHEMCAD. The MCsets listed in the MCPoints and used by the MCI procedure may be obtained by any random number program. For this work the sets were obtained with the same FORTRAN subroutines used for the FORTRAN versions of the OPT and CMCI procedures. The sets were saved in a text file using FORTRAN code. Later the file was opened using EXCEL and the information was copied and pasted on the EXCEL sheet MCsets.

Table A.21. List of subroutines and functions coded in the EXCEL/VBA environment for the OPT and CMCI procedures.

Subroutine or function	Description
AxialRadDir	Sets initial axial radial direction to search for BP's.
bipposinvectorsub	Sets element positions of BIP's in vector of uncertain parameters.
bndry	Calculates tangent and connecting planes.
BPSearch	Searches for BP's in certain radial directions.
checkconvba	Checks convergence of the NNG's.
Clear_BPCRD_Results	Clear summary of results from the BP search in sheet DataResSum.
Clear_Cells_Done	Clears word in cells in sheet DataResSum.
Clear_CMCI_DREResults	Clear summary of results from CMCI in sheet DataResSum.
Clear_ComponentsTrayEffAndBIPS	Clear components, tray efficiency and BIP's data in sheets DataResSum and BIPsStatDes
Clear_MSCS_Results	Clear summary of results from MS's in sheet DataResSum.
Clear_OPT_DREResults	Clear summary of results from OPT procedure in sheet DataResSum.
ClearCellDone	Clear word in cell.
CMCI	Main subroutine for running CMCI integration.
CompStreamsCCObj	Reads components, stream numbers and set CHEMCAD objects for later computations.
ConstReadInfo	Reads constraints information from sheet DataResSum.
ConvFarToRan	Converts temperature from Fahrenheit degrees to Rankin degrees.
ConvRanToFar	Converts temperature from Rankin degrees to Fahrenheit degrees.
FeedOption1	Flashes feed stream at given pressure to compute bubble temperature. Also computes enthalpy.
inchck	Checks if MC set is the space of the NNG.
incon2	Checks if MC set is inside connecting plane of NNG.
inconn	Control subroutine to check if MC set is inside connecting plane of the NNG.
IniStreamDat	Subroutine that control reading feed stream data, computing feed stream flash and displaying results in sheet DataResSum.
intan	Checks if the MC set is within the tangent-plane of the NNG.

Table A.21. (Continuation.)

Subroutine or function	Description
LabelingNew	Writes labels in CMCIRes sheet.
LabelsBPSearchPrepare	Writes labels in BPsSearch sheet.
LabelsMSPrepare	Writes labels in MSsCom sheet.
LineSearch	Computes Line-Search procedure.
LoadCC5	Connects Excel with CHEMCAD.
mcintg	Controls MCI computations.
mcintglast	Computes MCI with the last NNG's matrix and writes results in OPTRes sheet.
mcintgloop	Computes MCI.
ModelSimulation	Computes MS's for specified sets of parameter values.
neigha	Add a new BP to the NNG matrix.
neighb	Calculates hyperplanes that make up the boundaries of a NNG.
neighd	Determines in which quadrant a new BP is in.
neighd0	Enumerates the initial NNG's.
neighi	Initializes the NNG matrix.
neighp	Computes connecting-planes of NNG's.
neighs	Checks if each NNG has the same common active constraint
neight	Determines the type of curvature of the NNG's.
neighw	Controls the search of the NNG in which a MC set falls in.
nxtrad	Computes the next radial direction to search.
perturbparameters	Computes set of parameters in the search of BP.
readbips	Reads BIP's from CHEMCAD project and displays values in message boxes.
readNDBIPs	Reads BIP's data in CHEMCAD project and writes the data in sheet BIPsStatDes.
readNDtrayeff	Reads tray efficiency value in CHEMCAD and writes it in sheet DataResSum.
sdvdst	Calculates the distance of the radial vector in terms of the maximum step.
SetControlVariables	Reads control variables data from EXCEL sheet and sets values in CHEMCAD project
SetNominalUnitopSpec	Reads nominal design specifications from EXCEL sheet, sets values in CHEMCAD sheet, instructs CHEMCAD to run model simulation and displays results on EXCEL sheet DataResSum.

Table A.21. (Continuation.)

Subroutine or function	Description
TanApprox	Main subroutine to run the OPT procedure.
tanclc	Checks if a MC set is inside or outside a tangent plane.
UncSettings	Reads from sheet DataResSum number and type of uncertain parameters and sets counters.
UnloadCC5	Stops connection with CHEMCAD.
uno	Sets value of one in all the elements of a vector.
WriteDone	Write word "Done" in the specified cell.
writeNDBIPs	Reads BIP data (mean values) from sheet BIPsStatDes and writes data in CHEMCAD.
writeNDtrayeff	Reads tray efficiency from ChemCAD and writes it in DataResSum sheet.
zero	Sets value zero in all the elements of a vector.
zero2	Sets value of zero in all the elements of a matrix of specified dimensions.

Before loading CHEMCAD or running the OPT or CMCI computations a CHEMCAD project with the distillation column flow sheet of the case study must exist. The list of components is read by the VBA code from the CHEMCAD project and written on the DataResSum sheet.

To run the OPT or CMCI procedure the user may run the initial steps one by one sequentially:

1. Load CHEMCAD.
2. Initial feed stream data.
3. Set nominal specifications and run nominal case.
4. Set control variables.

Then the OPT PDR may be computed by pressing the button OPT DRE or the CMCI by pressing the button CMCI. Or the user may choose to do the complete computation by just clicking the OPT DRE button or the CMCI button by selecting to run the initial steps in cells B58 for the OPT procedure and cell F58 for the CMCI procedure.

For the CMCI procedure, the progress of the computations can be seen in the cell range F62 to F71 of the EXCEL sheet DataResSum. Results for each MC set are displayed in the EXCEL sheet CMCIRes. For the OPT procedure, the progress of the computations can be seen in the cells located under the cell B62 in the EXCEL sheet DataResSum. More detailed results can be found in the EXCEL sheet OPTRes.

The CHEMCAD projects and EXCEL files with the results for the case studies presented in this work are included in the attached CD under the directory EXCELIntegration.

A.5. SMSD in Visual C++ for coupling with CHEMCAD

The code for the SMSD procedure coupled with CHEMCAD was developed using mixed programming in the Visual C++ 6.0 environment. Compaq Visual FORTRAN 6.0 was used for creating a FORTRAN DLL that is used by the Visual C++ code.

The main code, which links the SMSD procedure with CHEMCAD, was developed using the Visual C++ DLL workspace provided by CHEMCAD. To avoid recoding in C++ some of the subroutines of the SMSD FORTRAN program, those subroutines were copied into a Visual Compaq DLL workspace to make them available to the Visual C++ code. Table A.22 lists the C++ functions that contain the code that was developed and a brief description of them. The list of FORTRAN subroutines contained in the FORTRAN DLL is presented in Table A.23.

Table A.22. List of C++ functions coded in the Visual C++ environment.

Function	Description
add6	Takes from the UAM add6's dialog boxes parameter uncertainty and flow sheet topographic information and passes it to the other modules. Controls the addition of BP's to the NNG matrix, i.e. external loop of the SMSD procedure computations.
add7	Controls the flow of the computations to approximate the CB.
add8	Compute the component feed flow rate values to be used in the search of a BP and flashes the feed stream. Together with function add9 control the search for BP's.
add9	Uses the results from the distillation column simulation to compute the constraint residuals to determine if the search for a BP has converged or if continue looking for a BP. Controls together with function add8 the search for BP's.
neighi	Initializes the NNG matrix.
inineighd	Enumerates the initial NNG's.
readbp	Reads the new BP information from file NewBP.txt . Then creates file BoundaryPoints.txt and saves the information.
readnewbp	Reads the new BP information from file NewBP.txt and adds this information to file BoundaryPoints.txt.
bndary2	Saves initial boundary information in file !BndryInfo.
bndary3	Saves (overwrites) boundary information in file BndryInfo2.txt.
bndary4	Saves (overwrites) boundary information in file BndryInfo4.txt.
intpow	Computes and return the value of an integer number raised to the specified power exponent.
mcres	Saves MCI results and real computing time in file !BndryInfo.
bappcrit	Uses rules to set if convergence of the CBA of a NNG has been reached.
bappcritcheck	Checks if convergence of the CBA of all the NNG's has been reached.
flashfeeds	Computes isothermal flash of the feed.

Table A.23. List of FORTRAN subroutines coded in the DLL FDLLUAM7.dll

Function	Description
NEIGHB	Calculates the hyper-planes that define the space of each NNG.
NEIGHP	Computes connecting-planes of NNG's.
MCINTG	Computes MCI.
NXTRAD	Computes the next radial direction to search for BP.
NEIGHA	Adds a new BP to the NNG matrix.

To run the SMSD procedure coupled with CHEMCAD it is necessary to have CHEMCAD version 5.6.4 installed. Also it is necessary to copy the files listed in Table A.24 in the CC5 directory. These files are included in the attached CD under the

directory SMSDCC5Files. The CHEMCAD projects for the case studies of this work are included in the attached CD under the directory SMSDCHEMCADProjects.

Table A.24. List of files that need to be copied to the CC5 directory .

File	Description
USRADD.dll	C++ DLL that contains the code for executing UAM's ADD6, ADD7, ADD8 and ADD9.
FDLLUAM7.dll	FORTRAN DLL that contains subroutines necessary for the MCI
$add6.lab	Defines CHEMCAD report labels and format for the UAM dialog box variables.
$add7.lab	Defines CHEMCAD report labels and format for the UAM dialog box variables.
$add8.lab	Defines CHEMCAD report labels and format for the UAM dialog box variables.
$add9.lab	Defines CHEMCAD report labels and format for the UAM dialog box variables.
ADD6.map	Defines the dialog box data array.
ADD7.map	Defines the dialog box data array.
ADD8.map	Defines the dialog box data array.
ADD9.map	Defines the dialog box data array.
add6.my	Define the visual aspect of a dialog box for input/output of the module data array.
add6_2.my	Define the visual aspect of a dialog box for input/output of the module data array.
ADD7.my	Define the visual aspect of a dialog box for input/output of the module data array.
add8.my	Define the visual aspect of a dialog box for input/output of the module data array.
add9.my	Define the visual aspect of a dialog box for input/output of the module data array.

To start the simulation computations of any of the provided CHEMCAD projects, it is necessary to reset the value of the number of iteration to zero in the General box dialog of module ADD6. The maximum number of iterations may be set to different value if desired. Then run the simulation of module ADD6. When CHEMCAD displays that the simulation is done, then click in the icon for running the full flowsheet simulation, i.e. the Run All icon. The simulation generates the output files listed and described in Table A.25

Table A.25. List of output files from the SMSD UAM's.

File	Information
BndryInfo.txt	Initial CBA equations, MCI statistics after each iteration of the procedure and computing time.
BndryInfo2.txt	CBA equations before the last BP was added to the NNG matrix.
BndryInfo4.txt	CBA equations after the last BP was added to the NNG matrix.
BoundaryPoints.txt	BP's, gradients and MS's.
comptime.txt	Initial time and time after each MCI is performed.
NewBP.txt	Intermediate file with BP('s) information.
newradial.txt	Radial direction(s).
resadd9.txt	Line-search procedure's results for each BP search.

References

MacDonald, R. J., 1993. An Accurate and Efficient Procedure for Estimating Design Reliability, Ph.D. Thesis, University of Kansas.

APPENDIX B

Property data for distillation column case studies

B.1. Property data for FORTRAN programs

The thermodynamic database model used the TK Wilson model for the liquid phase and the ideal gas law for the vapor phase. The BIP's for the TK Wilson model are provided in Table 2.1.

The component vapor pressure is modeled by the Miller equation.

$$\ln\left(P_i^{sat}\right) = \frac{A_i}{T} + B_i + C_i T + D_i T^2 \qquad \text{(B.1)}$$

where T is the temperature in degree Kelvin and P_i^{sat} is the component vapor pressure in kPa. Coefficient values for the components used in this work are listed in Table B.1.

Table B.1. Coefficient values for the Miller equation vapor pressure (MacDonald, 1993).

Component/ Coefficient	A	B	C	D
Acetone	-5.00E+03	2.60E+01	-2.55E-02	2.05E-05
Benzene	-5.39E+03	2.67E+01	-2.61E-02	1.94E-05
Water	-6.44E+03	2.79E+01	-2.19E-02	1.51E-05
Toluene	-5.92E+03	2.71E+01	-2.51E-02	1.72E-05
2-Methyl-1-Butene	-4.36E+03	2.46E+01	-2.51E-02	2.10E-05
Isoprene	-4.09E+03	2.17E+01	-1.56E-02	1.09E-05

Vapor and liquid enthalpies are modeled by third order polynomial curve-fit with ideal mixing. Table B.2 and B.3 provides the constants obtained by MacDonald (1993) and used in this work for liquid and vapor enthalpy, respectively.

The liquid solution model requires liquid molar volumes for each component. The Hankinson-Thomson correlation was used. Table B.4 lists the characteristic volumes for each component.

Table B.2. Coefficient values for the liquid enthalpy model (MacDonald, 1993).

Component/ Coefficient	A	B	C	D
Acetone	-1.74E+02	4.79E-01	1.56E-04	2.62E-07
Benzene	-1.33E+02	3.47E-01	2.48E-04	3.66E-08
Water	-3.16E+01	9.95E-01	9.74E-07	7.58E-08
Toluene	-1.37E+01	4.28E-01	0.00E+00	0.00E+00
2-Methyl-1-Butene	8.91E+02	4.80E-01	3.99E-04	1.91E-07
Isoprene	8.85E+02	4.72E-01	3.21E-04	3.12E-07

Table B.3. Coefficient values for the vapor enthalpy model (MacDonald, 1993).

Component/ Coefficient	A	B	C	D
Acetone	6.99E+01	2.68E-01	2.29E-04	-4.47E-08
Benzene	6.07E+01	2.08E-01	2.88E-04	-7.37E-08
Water	1.07E+03	3.63E-01	5.49E-04	-1.77E-06
Toluene	1.76E+02	2.27E-01	2.79E-04	-6.95E-08
2-Methyl-1-Butene	1.06E+03	3.13E-01	3.27E-04	-7.33E-07
Isoprene	1.06E+03	3.04E-01	3.10E-04	-6.73E-07

Table B.4. Characteristic volumes for Hankinson-Thomson correlation (MacDonald, 1993).

	Acetone	Benzene	Water	Toluene	2-Methyl-1-Butene	Isoprene
$\frac{cm^3}{gmol}$	-5.00E+03	-5.39E+03	-6.44E+03	-5.92E+03	-4.36E+03	-4.09E+03

B.2. Property data used with CHEMCAD

The programs coupled with CHEMCAD use CHEMCAD thermodynamic methods. For all the case studies the TK Wilson model was selected. For liquid densities the CHEMCAD library equation was selected. Latent heat was selected as the option for the global enthalpy and DIPPR for the ideal gas heat capacity.

B.3. Experimental data for regressing UNIQUAC parameters

Table B.5 lists the TPxy experimental data used for regressing the UNIQUAC parameters used in the safety factor analysis presented in Section 4.8. The data set was obtained from Gmehling, and Onken, (1977ff). Gmehling, and Onken, report that the data set was measured by Kooner and Fenby at 25 . ^{o}C and that it is thermodynamically consistent.

Table B.5 TPxy methanol/ethanol experimental data (Gmehling, and Onken, 1977ff) .

58.95	0.0000	0.0000
61.73	0.0431	0.0860
66.32	0.1129	0.2112
75.99	0.2564	0.4230
79.72	0.3110	0.4903
84.88	0.3879	0.5752
86.68	0.4135	0.6011
91.54	0.4843	0.6678
96.46	0.5563	0.7288
97.04	0.5654	0.7360
100.89	0.6206	0.7782
102.44	0.6437	0.7949
108.32	0.7296	0.8528
115.25	0.8303	0.9131
124.54	0.9656	0.9836
126.88	1.0000	1.0000

References

Gmehling, J. and Onken, U., 1977ff. Vapor–Liquid Equilibrium Data Collection. DECHEMA Chemistry Data Series, Frankfurt, Germany.

MacDonald, R. J., 1993. An Accurate and Efficient Procedure for Estimating Design Reliability, Ph.D. Thesis, University of Kansas.

APPENDIX C

Review of the literature

Uncertainty is an inherent characteristic of any process system. Overdesign using safety factors compensates for uncertainties.

C.1. Classification of process design uncertainties

Pistikopoulos (1995) classifies uncertainty in a process as follows:

1. Model-inherent uncertainty.
2. Process-inherent uncertainty.
3. External uncertainty.
4. Discrete uncertainty.

Pistikopoulos (1995) does not mention uncertainty due to the imprecise knowledge of the equipment operation (e.g. tray efficiencies, flooding points and heat transfer coefficients).

C.2. Description of process design uncertainties

In general, uncertainties are typically described as either probabilistic or possibilistic. Even some system aspects that are clearly deterministic, such as the periodic variations in temperature through the course of a 24-hour day can be characterized using probabilistic methods (Robinson, 1998). This dissertation focuses on probabilistic descriptions. For more details about its application refer to MacDonald (1993), Kubic and Stein (1986, 1988), Dubois et al. (1992), Grabisch et al. (1995), Sebastian and Antonsson (1996), Bezdek (1993), Kraslawski and Nyström (1994), and de Cooman et al. (1995).

C.2.1. Min/max bounds

The simplest type of uncertainty representation is minimum and maximum bounds for the value of the uncertain parameter. Since a minimum of information is required, they have been used in most of the historical development of design under uncertainty. However, there are major limitations with this representation:

1. It is often difficult or impossible to obtain precise values for these bounds.
2. Any additional information, such a "best estimate" or most likely value, cannot be used.

C.2.2. Probability distributions

Probabilistic techniques are characterized by random variables to describe the various sources of uncertainty and are generally referred to as reliability methods. These techniques are typically applied when the system under consideration is of small to moderate complexity (100-150 random variables or less) and is reasonably well understood (Robinson, 1998). Probability statistics are the most powerful uncertainty representation (MacDonald, 1993).

Some specific situations in which probability statistics cannot cope are:

1. Min/max bounds are sometimes all that is known.
2. Process simulation model errors are systematic, not random, which makes them very difficult to describe using probability distributions.
3. Empirical models must frequently be extrapolated into unknown regions, where it

is generally impossible to quantify the uncertainties.

C.3. Effects of uncertainty in process design

In the design of a chemical process, if the inputs describing a system are uncertain, the prediction of the performance of the process is necessarily uncertain (Xing and Whiting, 2000). The quality of the results depends of the quality of the inputs and the accuracy and precision of the model parameters. All model parameters, pure component data and binary, ultimately are determined from some form of experimental data. Then, the random and systematic errors inherent in experimental data affect the final design.

Early studies to demonstrate the consequences of bad thermodynamic data and inaccurate models were reported by Zudkevitch (1980), Howat (1983), Nelson et al. (1983), Macchietto et al., (1986), Larsen (1986) and Zeck (1991).

Whiting and coworkers (Whiting and Tong, 1993; Whiting, 1996; Vasquez and Whiting, 1998, 1999, 2000; Whiting et al, 1999; Xin and Whiting, 2000) have presented several studies to show the sensitivity of computer aided design to inaccuracy and uncertainty in thermodynamic data and models, and the uncertainty induced from the use of certain simulators. Several of these studies use Monte Carlo simulation to evaluate the uncertainty in the performance of the process. The uncertainty (accuracy and precision) in the design data must be known so that the effects in the final design can be understood and used in assessing the quality of the design. The remaining questions are:

1. How can the design engineer estimate the quality of the design with respect its ability to operate feasibly in the presence of uncertainties?

2. What is an efficient procedure that the designer engineer can use to conduct studies that aid him in the selection of safety factors to provide maximum benefit at a minimum cost?

C.4. Definitions

To accomplish a design objective, e.g., perform a chemical separation, a mathematical model of the process with its constraints must be developed and solved. The basic model that is assumed in this work involves the vectors of variables and parameters listed in Table C.1.

Table C.1. List of vectors of variables and parameters.

Vector	Definition
$\vec{x}$	State variables that define the system (e.g., flows, temperatures).
$\vec{d}$	Design variables correspond to the structure and equipment sizes of the process and fixed operating conditions (e.g., steam and cooling water temperature).
$\vec{z}$	Control variables that can be adjusted during the operation (e.g., flows, loads, utilities) to meet process specifications.
$\vec{\theta}$	Continuous uncertain parameters (e.g., inlet conditions, thermodynamic database).
$\vec{y}$	Integer uncertain parameters (considered in section C.1 as discrete uncertainty).

To keep simple the notation the vectors of the state, design and control variables, and uncertain parameters will be represented simply by x, d, z, θ, y.

A chemical process or an entire flowsheet with its specifications and constraints can be modeled in terms of variables and parameters by

$$h_m(x, z, \theta, d, y) = 0, \quad m \in M \tag{C.1}$$

$$g_l(x, z, \theta, d, y) \le 0, \quad l \in L \tag{C.2}$$

where C.1 equalities represent the steady state model equations or performance equations, e.g. material and energy balances, thermodynamic and kinetic equations. C.2 inequalities, constraint equations, represent process constraints that must be satisfied for feasible operation, e.g. physical constraints, minimum purity specifications, flooding limits in a distillation column, temperature and pressure within acceptable equipment operating ranges, maximum pumping rates. Note here that the vector of discrete uncertain parameters may not be present in all the design problems reported in the literature.

The designer sets the design variables and the unknowns to be solved are the state variables (e.g. temperature, pressure, composition), which have the same dimensions as the set of equalities. Most operations have control variables or operating degrees of freedom, these are controlled by the operator and can be varied within certain limits to optimize process operation or to meet the specifications and constraints, e.g. control variables for distillation might consist of column pressure, distillate rate. Finally, the process model is uncertain due to physical property database uncertainties and imprecise knowledge of the equipment operation. Also, the design problem itself might be uncertain, with imprecisely known feed stream compositions and economic factors. These process uncertainties are represented by parameters. These parameters are constants which instead of being a single value, are described by a range of values such as min/max bound or statistical distributions The design is developed at a single set of parameters, at the nominal design condition. To guarantee a larger range of feasibility of the design, the region of success can be increased by spreading the constraint boundaries away from the nominal design condition. This is accomplished by adding safety factors

to the design. Since overdesigning equipment is expensive, the effectiveness of any safety factor used can be evaluated by the impact that it has on the constraint boundaries.

C.5. Analysis of process design under uncertainty

It is important for a design engineer to be able to quantify the ability of a process or a complete flowsheet to be operated feasibly (success region) in the presence of uncertainties and to have a systematic method to aid in the selection of safety factors.

Table C.2 presents a summary of key contributions in the development of methods for designing chemical processes under uncertainty.

Essentially these developments can be classified in three categories:

1) Deterministic cases, where the uncertain parameters are described through sets of min/max bounds on their values.
2) Stochastic cases, where the uncertain parameters are described through probability distributions.
3) Possibilistic cases, where the uncertain parameters are described through possibility distributions or inclusive hybrid cases where some of uncertain parameters are described using possibility distributions and the others using probability distributions.

The techniques that have been applied in these developments to solve the problem of designing under uncertainty include: optimization techniques combined with other mathematical techniques, Monte Carlo simulation, possibilistic techniques, and mathematical techniques to approximate the constraint boundary region (feasible region). A discussion of these developments follows.

Table C.2. Literature in process design under uncertainty (based on list reported by Bansal et al 2002).

Authors	Key Features
Grossman and Morari (1983)	Review of flexibility analysis and design problems.
Halemane and Grossmann (1983) Ostrovsky et al. (1994, 1997, 2000)	Feasibility test; design for fixed degree of flexibility. Bounding algorithms for the problems considered by Halemane and Grossmann (1983).
Swaney and Grossmann (1985a,b) Kabatek and Swaney (1992)	Flexibility index; vertex enumeration algorithms. Improved implicit vertex enumeration algorithm.
Chacon-Mondragon and Himmelblau (1988, 1996) Ierapetritou (2001) Goyal and Ierapetritou (2002) Banerjee and Ierapetritou (2002)	Alternative metrics to those of Grossmann et al.; based on the proportion of feasible controls. Alternative metric based on the volume of the convex hull within the feasible operating region. Inner and outer approximation of the feasible region using simplicial approximation. Feasible region mapping using high-dimensional model reduction.
Grossmann and Floudas (1987) Floudas et al. (1999) Raspanti et al. (2000)	Active constraint strategy; MINLP formulation for feasibility test and flexibility index problems. Global optimization for the formulations of Grossmann and Floudas (1987). Smoothing of the MINLPs of Grossmann and Floudas (1987) using constraint aggregation.
Pistikopoulos and Grossmann (1988a,b) Pistikopoulos and Grossmann (1989a,b) Varvarezos et al. (1995)	Retrofit design for linear systems; analytical expressions for flexibility index. Extension to special classes of nonlinear systems. Flexibility index and retrofit design for linear systems using sensitivity analysis.
Howat (1983) Kubic and Stein (1988) MacDonald (1993)	Estimation of process design reliability using CMCI. Estimation of process design reliability using probability and fuzzy sets. Estimation of process design reliability using constraint boundary mapping.
Pistikopoulos and Mazzuchi (1990) Straub and Grossmann (1990) Straub and Grossmann (1993) Pistikopoulos and Ierapetritou (1995) Rooney and Biegler (1999)	Stochastic flexibility of linear systems with normally distributed parameters. Stochastic flexibility of linear systems with generally distributed parameters. Stochastic flexibility of nonlinear systems. Design and simultaneous evaluation of stochastic flexibility of nonlinear systems. Uses MINLPs formulation of Grossmann and Floudas (1987). Incorporates joint confidence regions and discretizes the uncertain parameters to accelerate the convergence.
Bansal et al. (2000) Bansal et al. (2002)	Parametric programming framework for feasibility test, flexibility index, design optimization, and stochastic flexibility of linear systems. Parametric programming framework for feasibility test, flexibility index, design optimization, and stochastic flexibility of linear convex and nonconvex, and nonlinear systems.

C.5.1. Deterministic cases

The main drawbacks of the approaches that use the min/max bounds description of uncertainty are:

1. Only min/max bounds can be handled. However, in many real-world applications data are usually available which allow a better definition of uncertainty in a statistical sense.
2. Min/max bounds might be uncertain themselves. Changing these bounds requires the full calculation to be repeated.
3. The final knowledge is limited. In the case of the feasibility test (estimated based on the parameter or control space), either the design is guaranteed to work, or it might fail. With regard to the flexibility index: it provides a conservative estimate of the inherent flexibility in a process design (Pistikopoulos and Mazzuchi, 1990); and it is not unique, changes in the inactive constraint can be made without affecting the flexibility index (Kubic and Stein, 1988; Ierapetritou, 2001).
4. The solution of the feasibility test is extremely difficult, since it is an infinite, non-differentiable, nonlinear programming, optimization problem. The main problem is identifying which set of parameters is the worst case. This critical or limiting condition of feasibility is often not obvious. It can occur at any extreme or vertex point of the parameter range or it can occur at any intermediate point (Grossmann and Floudas, 1987). Even assuming that the worst case is at one of the vertices, which is only valid for the linear and convex cases (Swaney and Grossman, 1985a,b; Grossman and Floudas, 1987), an exhaustive search may be prohibitively expensive in practice, since the number of optimizations problems

that must be solved increases exponentially with the number of uncertain parameters.

C.5.2. Stochastic cases

Approaches using probability distributions to describe parameter uncertainty measure the probability that the design will meet all the process constraints despite the underlying parameter uncertainty (stochastic flexibility or design reliability). Mathematically this is equal to the integration of the parameter joint probability distribution throughout the design's feasible region. The main drawbacks of these approaches are:

1. Approaches that use optimization techniques have the same mathematical difficulty discussed for the deterministic cases or are limited to linear systems.
2. Approaches using Cartesian products and conventional Monte Carlo integration as the integration technique are computationally too expensive.
3. Upper and lower bounds for the design reliability that may be too wide to be useful.
4. The constraint boundary mapping approach is computationally efficient (MacDonald, 1993), however it is not available to the design community.

C.5.3. Possibilistic case: fuzzy reliability

Fuzzy design reliability measures the possibility that there is some realization of the parameters in the fuzzy set of parameters for which the design works. Likewise, fuzzy design unreliability is the possibility that there is some realization of the parameters for which the design fails. The drawbacks of this approach are:

1. The fuzzy reliability is a nonlinear programming problem that may require expensive computational methods to be solved.
2. For the fuzzy unreliability only an upper bound is estimated using a heuristic procedure which accuracy is unknown.

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